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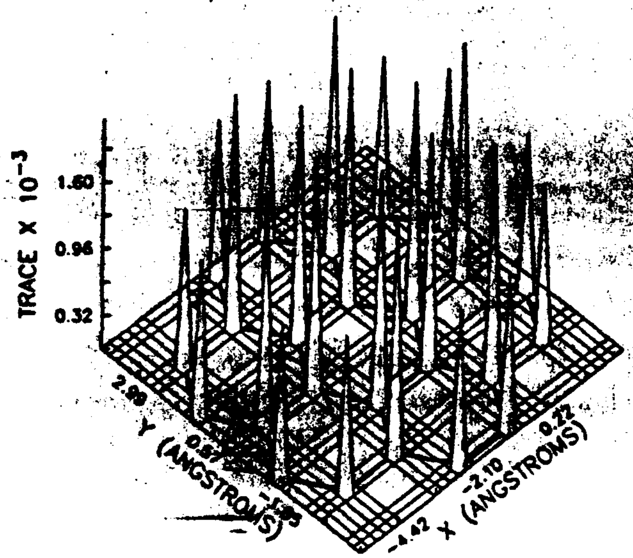
C.M.D.S.6

I. S. I. M. M.

6TH SYMPOSIUM ON CONTINUUM MODELS AND DISCRETE SYSTEMS

June 26-29, 1989
University of Burgundy
Dijon, France

ABSTRACTS



Traces of the elastic modulus tensor for a hexagonal planar array of carbon atoms (after Thacher et al, 1986).

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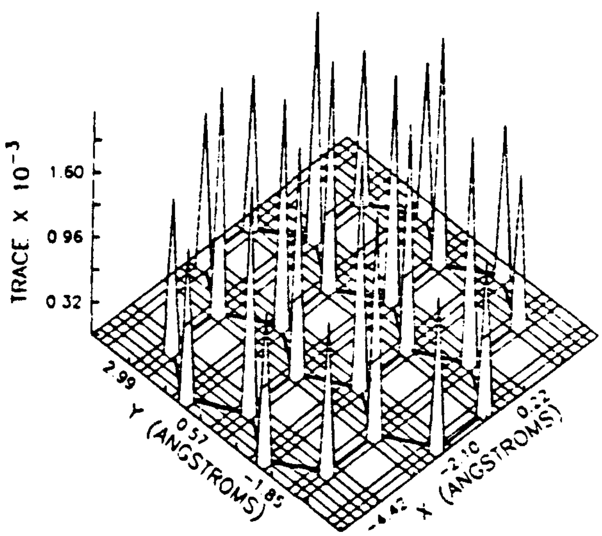

Traces of the elastic modulus tensor for a hexagonal planar array of carbon atoms (after Thacher et al, 1986).

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"... c'est l'ordre de grandeur qui, à lui seul, crée le phénomène. Si la longeur d'onde λ *n'était pas assez grande pour enjamber en quelque sorte les discontinuités de la distribution punctiforme, la confusion s'installerait ... La grandeur de la quantité* λ *relativement aux distances interatomiques ... détermine une solidarité qui calque la continuité".*

G. BACHELARD in : *Study of the Evolution of a Problem in Physics : Thermal Propagation in Solids.*
(Complement to *Doctorat d'Etat ès Lettres*, 23 mai 1927).

INTERNATIONAL SOCIETY FOR THE INTERACTION
OF MECHANICS AND MATHEMATICS

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1789 *1989*

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6TH SYMPOSIUM ON CONTINUUM MODELS AND DISCRETE SYSTEMS

Dijon, June 26-29, 1989

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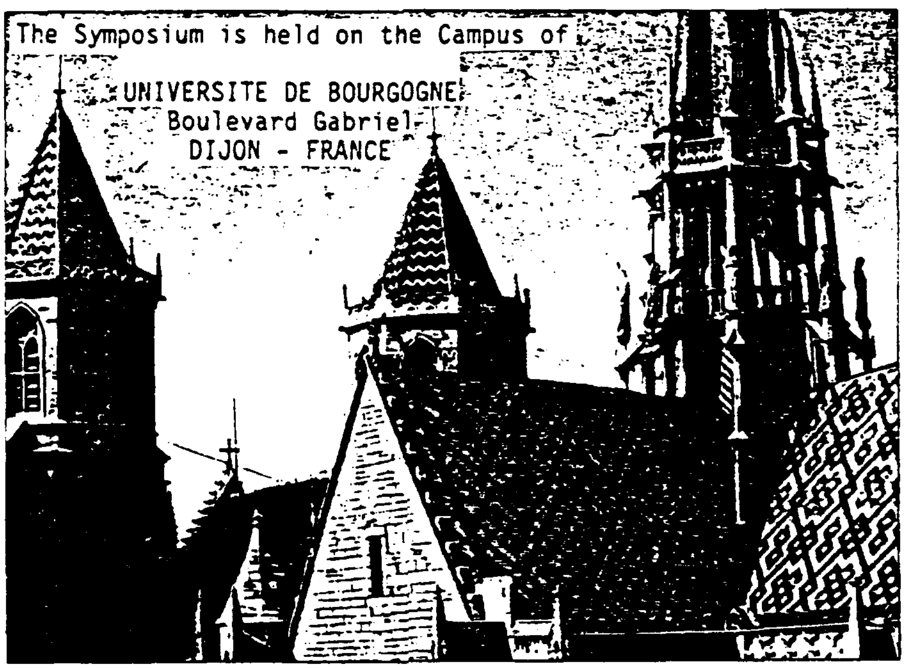

Placed under the auspices of the *International Society for the Interaction of Mechanics and Mathematics* and the *Association Universitaire de Mécanique* (France), the Symposium is organized with the financial aid of

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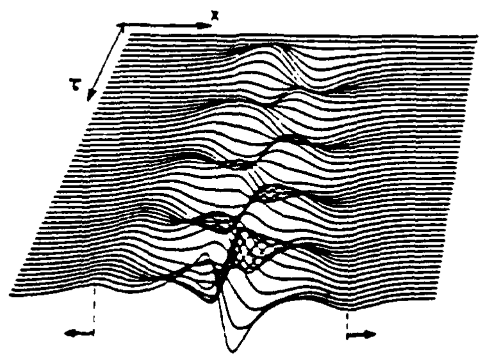

Some landmarks

1489 Christopher COLUMBUS thinks about his "west road" to India,

1689 The Bill of Rights, England,

1789 Birth of Augustin-Louis CAUCHY,

1829 A.-L. CAUCHY publishes his *"Sur l'équilibre et le mouvement intérieur des corps considérés comme des masses continues"*.

1839 George GREEN's *"On the Propagation of Light in Crystallised Media"*,

1869 Lord KELVIN publishes his paper *"On Vortex Motion"*,

1879 J. BAUSCHINGER describes the *"Bauschinger effect"*,

1889 W. VOIGT's *"Crystal Elasticity"*,

1909 C. CARATHEODORY publishes his *"Untersuchungen über die Grundlagen der Thermodynamik"*,
E. and F. COSSERAT publish their *"Théorie des corps déformables"*,
J.H. POYNTING announces the *"Poynting effect"*,

1919 H. BARKHAUSEN discovers the *"Barkhausen jumps"*,

1929 O. KELLOGG publishes his *"Foundations of Potential Theory"*,

1939 H.M. WEESTERGARD's *"Bearing Pressure and Crack"*,
H. WEYL publishes his *"Classical Groups"* at Princeton,
J.M. BURGERS' *"Some Considerations on the Fields of Stress Connected with Dislocations in a Regular Crystal Lattice"*,
J.F. FRENKEL and T. KONTOROVA publish their paper *"On the Theory of Plastic Deformation and Twinning"*,

1949 V. BARGMANN's *"On the Connection Between Phase Shifts and Scattering Potentials"*,
D. GABOR gives the principle of holography in his *"Microscopy by Reconstructed Wavefronts"*,
C.A. TRUESDELL's definition of Stokesian and Maxwellian fluids,

1989 CONTINUUM MODELS AND DISCRETE SYSTEMS 6, Dijon, France.

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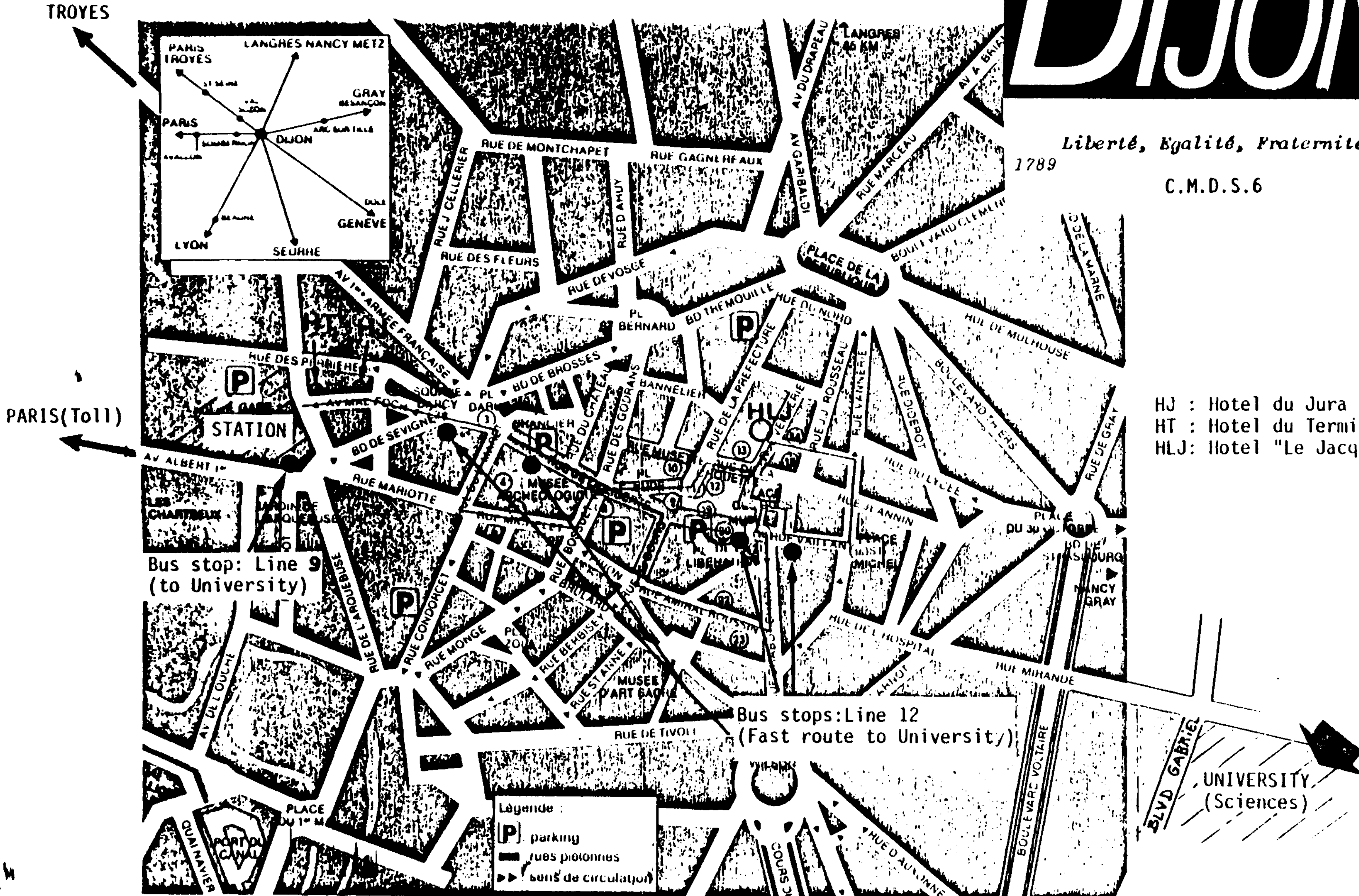

HJ : Hotel du Jura
HT : Hotel du Terminus
HLJ: Hotel "Le Jacquemard"

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UNIVERSITE DE BOURGOGNE

C.M.D.S.6

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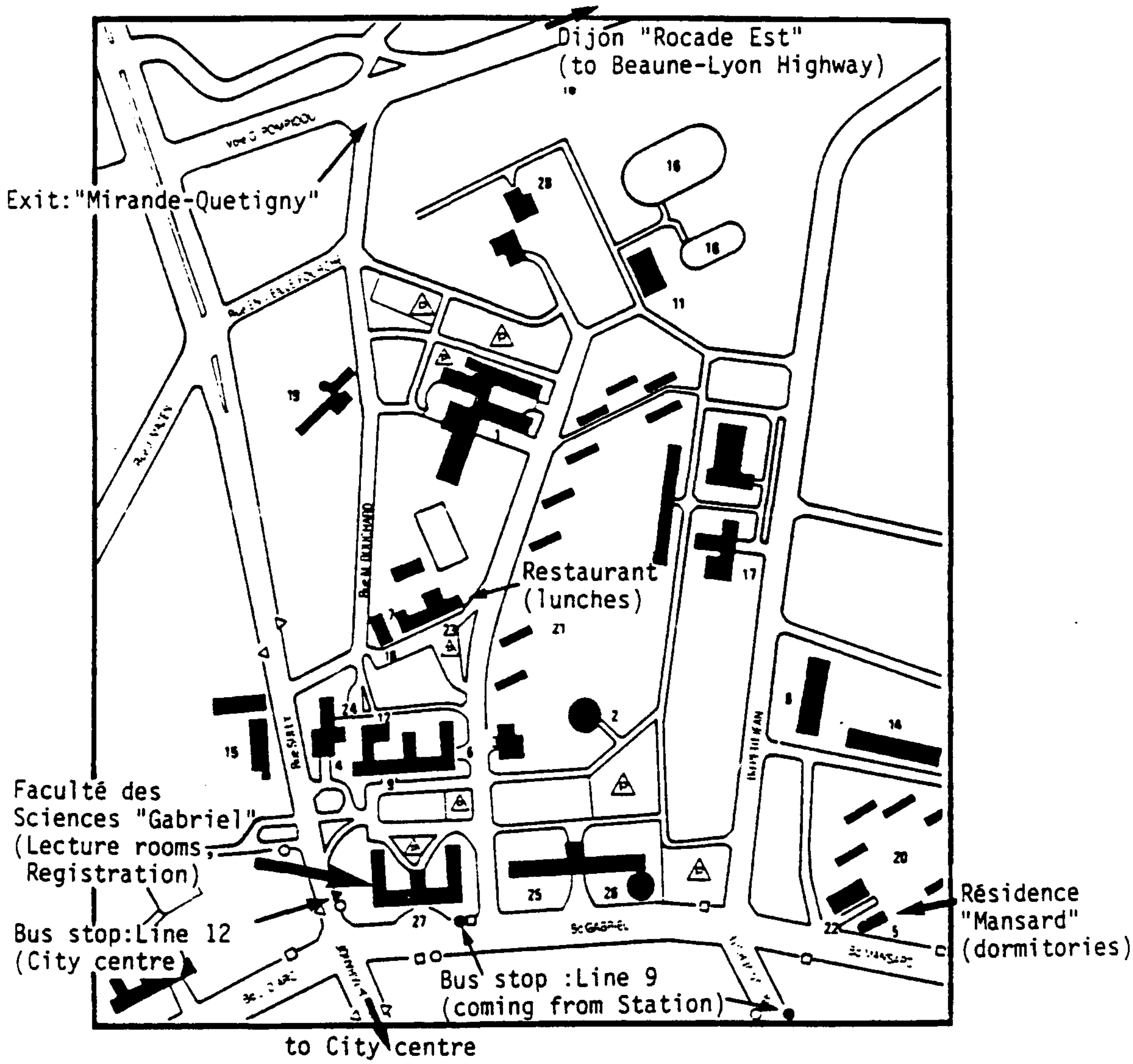

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18 Medecine Preventive
19 Residence Beaune
20 Residence Mansard
21 Residence Montmuzard
22 Restaurant Mansard
23 Restaurant Montmuzard
24 SIO
25 UFR juridiques et economiques
26 UFR litteraires
27 UFR scientifiques - Bt Gabriel
1 UFR scientifiques - Bt Mirande
28 UFR STAPS
29 Gymnase

Arrêts bus 21 9 12

Parkings

C.M.D.S.6.

SCHEDULE

	Monday June 26 A	Monday June 26 B	Tuesday June 27 A	Tuesday June 27 B	Wednesday June 28 A	Wednesday June 28 B	Thursday June 29 A	Thursday June 29 B
9.00-9.20	REGISTRATION		NL: HESS		NL: NAYFEH		NL: SIMO	
9.20-9.40								
9.40-10.00			NL: LENORMAND		NL: MARADUDIN		NL: ROGERS	
10.00-10.20	OPENING		BRIEGER	TELEGA	MAYER	SATAKE	PEYRARD	LITEWKA
10.20-10.40	NL: GRMELA		LHUILLIER	NOWACKI	PLANAT	PARTON	ASKAR	OSTOJA
10.40-11.00			BREAK		BREAK		BREAK	
11.00-11.20	NL: HSIEH		NL: BURRIDGE		NL: WILLIS		NL: CHERKAEV	
11.20-11.40	GOUIN	MARKOV						
11.40-12.00	KOTOWSKI	KUNIN	DOREMUS	LIMAT	REMUISSE-NET (NL)	ZAOUI	MUSCHIK	KUBIN
	LUNCH		LUNCH		LUNCH		LUNCH	
14.00-14.20	NL: LALLEMAND		EXCURSION		NL: TURSKI		NL: TREBIN	
14.20-14.40								
14.40-15.00	NL: FEUILLEBOIS				NL: POUGET		NL: KERNER	
15.00-15.20	BANACH	FAHNLE			CADET	PARRY	ANTHONY	WACK
15.20-15.40	PAPENFUSS	BERVEIL.			PARKER	HUET	MELEHY	TEODOSIU
15.40-16.00	BREAK				BREAK		BREAK	
16.00-16.20	NL: CHRISTOV				NL: SOBCZYK		NL: POMMARET	
16.20-16.40							CLOSURE	
16.40-17.00	NL: GOLDSHTIK				NL: MILTON			
17.00-17.20	MORRO	MAZILU			BRAUN	NAVI		
17.20-17.40	MURDOCH	MICUNOVIC			AL ASSAAD	DATTA		
17.40-18.00	STRAUGHAN	LEBLOND			MILOH			
EVENING	RECEPTION		RECEPTION		BANQUET			

NL = "nominated" lecture, A = Amphi "PASTEUR", B = Amphi B

1 indicates the topics

ABSTRACTS

OF

LECTURES AND CONTRIBUTED PAPERS

CMCSt-TIIN.1383

NONLINEAR WAVES IN LIQUID-GAS MIXTURES: AN ASYMPTOTIC THEORY

Al Ayham AL ASSA'AD and Jean-Sylvestre DARROZES

Groupe Phénomènes d'Interface
Ecole Nationale Superieure de Techniques Avancées
91120 Palaiseau-FRANCE

Abstract

Based on Eringen's micromorphic theory of continua [1,2], new local balance laws, constitutive relations, field equations and an equation of state for bubbly liquids with single velocity and temperature fields have been recently developed [3].

In this paper we consider the system of field equations which admits, in a linear approximation, a plane wave solution with high-frequency oscillation. For a wave of small but finite amplitude, we investigate how slowly varying parts of the wavetrain such as the amplitude are modulated by nonlinear interactions. The derivative-expansion method with multiple scales [4] is applied to the analysis of weak nonlinear waves propagating through the mixture. Its shown that the nonlinear Schrödinger equation can be derived from the condition that the perturbation expansion be free from secular terms. For long waves, a stretching transformation [5,6] shows that, in the lowest order of an asymptotic expansion, the original system of field equations of the mixture can be reduced to the Korteweg-de Vries equation.

References

[1] A.C. ERINGEN, "Simple micro-fluids", *Int. J. Eng. Sci.* **2**, 205-217, 1964

[2] A.C. ERINGEN & E.S. SUHUBI, "Nonlinear theory of simple microelastic solids. Part I.", *Int. J. Eng. Sci.* **2**, 189-202, 1964

[3] A. AL ASSA'AD & J.S. DARROZES, "Toward a continuum theory of liquid-gas mixtures", *Recent Advances in Engineering Science: the Eringen Symposium*, Berkeley, 1988

[4] A. JEFFREY & T. KAWAHARA, *Asymptotic Methods in Nonlinear Wave Theory*. Pitman, London, 1982

[5] C.H. SU & C.S. GARDNER, "Korteweg-de Vries equation and generalization III: Derivation of the Korteweg-de Vries equation and Burgers equation", *J. Math. Phys.* **10**, 536-539, 1969

[6] A. JEFFREY & T. KAKUTANI, "Weak nonlinear dispersive waves: A Discussion centred arround the Korteweg-de Vries equation", *SIAM. Rev.* **14**, 582-643, 1972

DEFECT DYNAMICS AND LAGRANGIAN THERMODYNAMICS OF IRREVERSIBLE PROCESSES

K.- H. Anthony
Universität Paderborn. Theoretische Physik. D 4790 Paderborn. FRG

Lagrange-Formalism (LF) of complex-valued fields applies to thermodynamics of irreversible processes (TIP). For heat transport, matter diffusion and chemical reactions I succeeded to verify this statement. The dynamics of topological defects in ordered materials, i.e. migration, creation, annihilation of defects and the reactions between defects of different types can be regarded as chemical reaction dynamics in a generalized sense. Thus in the framework of LF there emerges the perspective of a methodically unified continuum theory taking into account the tradtional continuum theory of topological defects as well as TIP. In my opinion such a unification is neccessary to take properly account of dissipation associated with defect dynamics. Within LF dissipation is associated with an irreversible energy transfer from kinematical and material degrees of freedom to thermal dgrees of freedom. This transfer is formally due to Noether's procedure which is a most important structure within LF.

Defect dynamics is a prominent example for the concept of internal variables in TIP. By means of LF I aim to take explicitly account of these internal variables, i.e. to avoid the concept of memory functionals which is used in rational thermodynamics. In LF these internal variables are realized by a set of complex-valued field variables each of which is associated with one particular type of defects. This set of "defect-fields" is supplemented by a complex-valued "field of thermal excitation". As compared with traditional TIP the set of fundamental field variables is doubled: The total amount of the complex-valued fields define defect densities and the temperature whereas the phase functions are physically associated with deviations from local equilibrium. By the "principle of local equilibrium" which is a prominent constraint in traditional TIP the processes are restricted to a sufficiently small neighbourhood of local thermal equilibrium. LF, however, suffers no restrictions of this kind. It allows for arbitrary dynamics even far away from local equilibrium.

Once a Lagrange-density-function depending on the defect fields and on the thermal excitation field is established the complete dynamics of the system is defined. By means of the well-known procedures of LF all field equations, balance equations and constitutive equations can be derived. Especially reactions between defects of different types are modelled by suitably coupling of the respective defect fields. This is done by means of a reaction potential which is an essential part of the Lagrangian and which takes account of the reaction dynamics of the defects on the atomic level. Quite generally it is an important feature of my Lagrangian approach to take account of the microscopic dynamics as far as possible.

CNDS6-DIJON,1989

DYNAMICS OF SINGLE HELIX AND DNA CHAINS:

Continuum and Discrete Analyses

Attila Aşkar

Bogazici Universitesi, Bebek, Istanbul, Turkey

The structure and the interactions between the particles forming the DNA double helix are described. In particular, the two particle stretching, the three particle bending and the four particle dihedral angle (or torsional) interactions along with the magnitudes of the energies involved are classified. The kinematic variables for each interaction are defined and the corresponding internal energy expressions are derived both for the discrete system and within the continuum representation. The dynamics of the globular state is mentioned briefly, while the emphasis is on isolated coils. Physical deductions are made for specific longitudinal and transversal modes for both a single and a double helix.

CMDS6-DIJON,1989

ON THE ANALOGUE OF GRAD'S MOMENT PROCEDURE FOR A ONE-DIMENSIONAL GAS OF QUASIPARTICLES

Z. BANACH
Institute of Fundamental Technological Research
Department of Fluid Mechanics
Polish Academy of Sciences
Swietokrzyska 21, 00-049 WARSAW, Poland

Let $\hbar\Omega$ be a quasiparticle energy attached to each value of the "wave number" k and suppose that $\Omega \propto |k|^{\nu}$, $1 < \nu \leq 2$. Within the framework of the Boltzmann-Peierls equation, we then extend the range of validity of Grad's moment procedure and, in fact, of the new method of one of our previous papers to the case of a one-dimensional gas of quasiparticles. Thus not without reason, an expansion with respect to k of the distribution function f around the local Bose-Einstein occupation probability f_0 in terms of the suitably chosen Tchebychef polynomials (Sansone's terminology) is carefully recognized. The importance of this representation in any serious analysis of equilibrium fluctuations in extended thermodynamics is clearly established. Characterizing a mesoscopic state of the quasiparticle system by a finite set $A^r_{-1} := (\alpha_0,\ldots,\alpha_r)$ of the first r $(r \geq 1)$ moments of f, we arrive in the course of linking thermodynamics (Müller's axiom of entropy growth) with kinetics, at the moment representation for f which is completely determined by the gas-state variables A^r_{-1}.

ON THE EFFECTIVE CONDUCTIVITY OF CRACKED BODIES
by

Y. Benveniste, Department of Solid Mechanics, Materials and Structures
T. Miloh, Department of Fluid Mechanics, and Heat Transfer
Faculty of Engineering, Tel Aviv University
Ramat-Aviv, Tel-Aviv, Israel

Several models are presented and discussed here for the effective thermal conductivity of cracked bodies containing aligned or randomly oriented cracks.

In the case of aligned cracks a microgeometry is constructed [1], which is a generalization of Hashin and Shtrikman's [2] composite sphere assemblage geometry, and consists of oriented elliptical cracks of all sizes. The effective thermal conductivity of this microgeometry is shown to possess an exact solution which can be cast in a surprisingly simple closed form. The significance of a crack density parameter for this model is discussed, and the derived effective conductivity is shown to fall below Willis's upper bound [3].

Recent results [4], [5] on cracked bodies with randomly oriented elliptical cracks are also briefly discussed. These include micromechanics modeling by the "generalized self-consistent scheme" and Mori-Tanaka's method.

[1] Y. Benveniste, and T. Miloh, submitted for publication.
[2] Z. Hashin and S. Shtrikman, J. Appl. Phys., 33, 1514, (1962).
[3] J.R. Willis, J. Mech. Phys. Solids, 25, 185, (1977).
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[5] Y. Benveniste, and T. Miloh, in Mechanics of Composite Materials, edited by G.J. Dvorak and N. Laws, ASME, AMD-Vol. 92, p. 87 (1988).

GRAIN SIZE EFFECTS IN POLYCRYSTALLINE PLASTICITY

M. BERVEILLER and A. SABAR
LPMM, UA CNRS 1215, ISGMP-ENIM
Faculté des Sciences, Ile du Saulcy
57045 METZ CEDEX, France

The granular structure of metallic polycrystals induces an additional hardening (with respect to the hardening of single crystals) due to the presence of grain boundaries.

At least three kinds of effect may be mentioned :

1) Plastic incompatibilities inducing long range internal stresses produce multiple plastic slips which lead to a supplementary isotropic and kinematic hardening with respect to single crystals. These phenomena are taken into account by the advanced models (like self-consistent or statistical) which deal with the internal stresses associated with interfacial or geometrically necessary dislocations. This is the case of models based on the solution of the plastic inclusion problem. Nevertheless, the grain size effect does not appear in such approaches.

2) The triple junctions between grains induce a non-uniform stress field inside the grains and contribute to the development of inhomogeneous plastic strain inside the grains. This rather complicated effect has to be dependent on the grain size but is not considered here.

3) At a minor scale, one may expect to observe a grain size effect associated with the fine structure of interfacial dislocations, reflecting the inhomogeneous deformation at grain boundaries (piles up...). The self-consistent modelling for which the plastic strain is homogeneous inside the grains, distributes the dislocations exclusively inside the grain boundaries (surface dislocations). This repartition may be acceptable if one wishes to evaluate the long range stress fields but does not take into account phenomena like piles up.

In order to take into consideration the fine structure of dislocations at grain boundaries, we suppose that the average mean free path of geometrically necessary dislocation decreases with increasing plastic strain. This decrease is evaluated using a very simple theory of dislocation piles up.

Next, the stress field for a plastic inclusion with mobile interface is given and used to build a model which incorporates both long range stresses (Kröner's model) and the (long range) stress due to piles up.

In this manner, the effects of grain size associated with the fine structure of the geometrically necessary interfacial dislocations are taken into account and give a polycrystalline hardening depending on grain size.

A FRENKEL-KONTOROVA MODEL WITH LONG-RANGE INTERACTION BETWEEN ATOMS

O.Braun, Yu.Kivshar and I.Zelenskaya

Institute of Physics, Kiev 252028, USSR

The statics and dynamics of kinks in a chain of atoms moving in a periodic potential with long-range repulsive interparticle interactions are studied. It is demonstrated that the dynamics of this model in the continuum approximation is described by an integro-differential equation which is an extended version of the sine-Gordon equation. The power law of a long-range interaction between kinks is determined. It is shown that the dependence of the Peierls energy for the kink versus the concentration of atoms in the chain takes the form of an Devil's staircase. Analytical results are in agreement with the numerical ones obtained by means of the molecular dynamics simulation. The theory can be applied to the surface diffusion of atoms along chains adsorbed on stepped or furrowed crystal surfaces.

ON THE INFLUENCE OF THE PHASE CONNECTIVITY ON THE YIELD POINT AND THE PLASTIC FLOW OF TWO-PHASE MATERIALS

by Thierry BRETHEAU, Eveline HERVE and André ZAOUI
Laboratoire des Propriétés Mécaniques et Thermodynamiques des Matériaux
CNRS / Université Paris-Nord - Villetaneuse (FRANCE)

Usual models are unable to deal with arbitrary space distribution of the phases of inhomogeneous random materials and are adequate only for very special situations (e.g. graded or perfect disorder). In the simple case of a two-phase Fe-Ag material, they fail to agree even with the prominent experimental results. Such a disagreement may be :

- qualitative : the observed existence of a concentration range where Lüders bands, which are characteristic of a Fe-like behaviour, can occur and propagate and its sudden ending at a critical (about 70 %) iron volume fraction cannot be predicted ;
- or quantitative : the stress-strain tensile curves in the concentration range where Lüders bands are no more present lie in a much lower position than it could be predicted by a classical self-consistent treatment.

It is experimentally observed and theoretically shown that the connectivity of one of the two phases is mainly responsible for these major experimental evidences :

- in the larger Fe volume fractions range, the connectivity of the iron phase makes it possible the propagation of the Lüders bands despite the presence of the inhibiting silver phase : it is proved, by use of a boolean stereological model which is identified on 2D-micrographs thanks to a picture processing analysis that the Lüders bands disappear when the connectivity number rapidly changes.
- in the larger Ag volume fractions range, the connectivity of the silver phase is responsible for an overall plastic behaviour which is "softer" than it would be predicted if both phases had equivalent morphological positions. On the contrary, the experimental observations are better modelled thanks to a restated and extended Christensen elastic-plastic "three-phase model" which deals with an iron-core and silver-shell composite spherical inclusion embedded in an effective material matrix.

Attention is focussed in conclusion on the merits of a new class of extended self-consistent models dealing with composite inclusions and illustrative applications of such models are mentioned.

A STOCHASTIC CELLULAR AUTOMATON MODEL OF DIFFUSION AND REACTION IN A POROUS MEDIUM

*Leesa Merle BRIEGER** and *Ernesto BONOMI***
*Department of Mathematics
**GASOV Group
Ecole Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

The model of diffusion provided by the random walk of a particle on a square lattice is driven by a simple rule: displace the particle with equal probability in any one of the four directions on the lattice. With this local rule we update the position of the particle at each time step, simulating its diffusive movement. The same rule, adapted to constrain at most one particle per site and applied individually to each member in a population of particles, reproduces diffusive motion in the population. Such a model, discrete in space and time, in which local or microscopic rules imposed on the individuals drive the macroscopic behavior of the system is a (stochastic) cellular automaton. This is our basis for an automaton model of diffusion and reaction in a porous medium, specifically the carbonation of concrete.

We compare two alternative implementations of the model: asynchronous and synchronous. In the asynchronous automaton only one particle at a time is randomly chosen from the population and allowed to move. The corresponding master equations which describe the evolution of the probability density have the form of the finite difference discretization of the diffusion equation. The asychronous automaton, then, reproduces just the solution of this discretized equation. The synchronous model, in which the entire population moves simultaneously, induces an interaction between particles due to the competition for free sites. The resulting master equations also have the form of the discretized diffusion equation but with an error term which we examine more closely in an investigation of Fourier's law.

Consider the diffusion equation $\frac{\partial u}{\partial t} = \mathrm{div}(D\, \mathbf{grad}(u))$ where the diffusion coefficient D can be a function of position and subject to spatial inhomogeneities. Benefitting from the local character of the automaton rules, we alter the particles' displacement probabilities and simulate the inhomogeneous diffusion. In a porous medium, various transport mechanisms, including capillary flow and molecular diffusion, are combined and modelled as effective diffusion. The resulting description is given by a diffusion equation of the above form, in which the effective diffusion coefficient D is a function of u, the solution. We reproduce this non-linear diffusion in the automaton and apply it in a study of drying in concrete, introducing physical units into the previously dimensionless model.

In the carbonation problem, carbon dioxide, CO_2, from the atmosphere enters concrete pores as they are emptied by drying. Calcium hydroxide, $Ca(OH)_2$, present in the concrete as a hydration product, reacts with the incoming CO_2 to form calcium carbonate, $CaCO_3$ and liberating water. The reaction decreases the pore water pH, threatening interior steel reinforcements with corrosion if ever it reaches them. Of interest, then, is the simulation of the inward progress of the reaction front.

Automaton rules can be augmented to increase the complexity of the physics simulated without changing the structure of the model. In a relatively simple expansion of the local rules of our automaton model, we define the dynamics of two diffusing species, two stationary species and the chemical reaction in a prototypical simulation of the full carbonation problem.

CMDS6-DIJON,1989

WAVES IN FINELY LAYERED MEDIA

Robert Burridge

Schlumberger-Doll Research
Old Quarry Road
Ridgefield, CT 06877-4108
U.S.A.

ABSTRACT

We consider an impulsive wave as it traverses a finely layered medium consisting of a large number N of homogeneous isotropic elastic layers. The directly transmitted wave is reduced by scattering loss at each interface and eventually becomes insignificant. However, close to the arrival of this direct wave is a broad pulse, arising from multiple scattering; this pulse does not decay as rapidly as the direct wave and ultimately appears to diffuse about a moving center. The latter process, which is determined by the medium statistics, leads to apparent attenuation, time delays, and apparent anisotropy.

We describe the work of Burridge, White, and Papanicolaou (1988) and Burridge and Chang (1989) and extend it to allow for tunneling P waves for S-wave incidence beyond the critical angle, and for a point source as opposed to plane waves. That work in turn is an extension of results described by O'Doherty and Anstey in 1971.

When the reflection coefficients at the interfaces are scaled as $1/\sqrt{N}$ while $N \to \infty$, and when time is measured in units of vertical travel time across an average layer, numerical solutions of the exact problem show that the shape of the broad transmitted pulse approaches the limiting form in accordance with the asymptotic theory. The same results could be obtained by combining ray theory with a modification of pulse shape governed by a certain integrodifferential equation.

Moreover, we find that travel times calculated by the effective medium theory and the theory her presented agree in a sense that will be made precise.

SOLITARY WAVES IN A MECHANICAL MODEL OF SHAPE MEMORY ALLOYS.

S. Cadet and G.A. Maugin
Laboratoire de Modélisation en Mécanique
Université P. et M. Curie, tour 66
4, place Jussieu, F75252 PARIS CEDEX 05, FRANCE

We present a discrete model of shape memory alloys which aims at reflecting the mechanical behaviour of these materials. The shape memory effect and related phenomena such as pseudoelasticity and ferroelasticity are due to a first order martensitic phase transition. The high temperature austenitic phase transforms into martensite variants or twins, mainly through a shear deformation parallel to the habit plane. However shearing is not the only deformation involved in the transformation: a small change in volume, usually less than 1%, is observed. The transition can also be induced by applying an external stress which favours one of the martensite variants. The coexistence of twins and of austenite with martensite results in domain boundaries which move when temperature or applied stress vary.

Starting from a discrete lattice model, we investigate the dynamics of nonlinear waves that are supposed to represent domain walls. We consider an atomic chain, of which each particle represents a crystal plane. Motion is allowed in the longitudinal direction as well as a transverse one, since transverse deformations are large; this could account for change in volume. The nonlinear equations of motion yield solitary wave solutions of several types. Kink solutions represent domain walls either between austenite and martensite or between two martensite variants. They move only when an external force is applied and obey a Rankine-Hugoniot equation. Pulse solutions correspond to a matrix of austenite or martensite containing a moving sheet of the other phase. The presence of longitudinal deformation and its coupling with transverse deformation affects strongly the stability of the various excitations. The results are illustrated by numerical simulations.

DISLOCATION MICROSTRUCTURES AND PLASTIC FLOW: A 3D SIMULATION

G. Canova[1] and L.P. Kubin[2]

[1] L.P.M.M. (UA CNRS 1215), Faculté des Sciences, Ile du Saulcy, 57045 Metz Cedex, France.

[2] L.E.M (CNRS-ONERA, OM), 29, Av. de la Division Leclerc, BP 72, 92322 Châtillon Cedex, France.

Numerical simulations of the arrangement of dislocations during plastic flow aim at investigating (i) the type of organization (walls, cells, slip lines and bands, various types of heterogeneities) obtained with different testing conditions (creep, monotonic deformation, fatigue...), (ii) its evolution with time or strain and (iii), its relation to the macroscopic, i.e. integrated, response of the simulated specimen. These methods present two advantages with respect to analytical elaborations: they are free from simplifying hypothesis and they reproduce accurately the elementary mechanisms of short and long range interactions between dislocations. They may also be used to elaborate macroscopic constitutive laws and to test the effect of various possible approximations at microstructural scale, such as e.g. a cutting off the long range elastic interactions or the introduction of an effective diffusion coefficient, as done within the so-called reaction-diffusion approach.

At present, only 2 D simulations have been developed, which necessarily involve some arbitrariness in the treatment of such processes as dislocation multiplication and which deal only with infinite, straight, dislocations of identical character (edge or screw) and of same Burgers vector. The 3 D simulation presented here is based on a discretization of space. Dislocation segments of edge and screw character lie on a tridimensional lattice, L, homothetic to the cristallographic lattice of the material considered (an F.C.C. crystal in the preliminary example described here). The lattice spacing a, associated with L, is defined through the shortest length scale needed to reproduce short range dislocations interactions. In the present case $a = 2y_c$, where y_c is the critical annihilation distance of an edge dipole under the influence of its self-stresses.

Segments of dislocations, of finite length, of edge or screw character and of any of the Burgers vectors available in the crystallographic structure considered, move by discrete steps according to a stress criterion. These segments are straight and both their lengths and their elementary translations are multiples of the lattice spacings of L. A dislocation loop, for instance, is represented by a succession of short screw and edge segments whose mutual interactions simulate the line tension. Local stresses are computed as the sum of applied (tensorial) stresses and internal (mutual interaction) stresses. Elementary mechanisms such as glide, cross-slip, climb, mutual annihilation, the formation of dislocation junctions are taken into account and other mechanisms such as dislocation multiplication, the cutting of repulsive trees, dipole trapping, follow naturally and need not be explicitely introduced.

The 3 D simulation method consists of following the segments themselves rather than the nodes of the lattice (this last procedure being closer to a classical automaton technique), and of coding the state of each segment in form of one integer. It is then possible to deal with dislocation densities up to $10^{15}\ m^{-2}$, in a crystal of $30x30x30\ \mu m^3$, with periodic boundary conditions. The total deformation may be controlled via the applied stress and a homogeneous lattice rotation takes into account the activity of the slip systems.

Preliminary results will be presented on a simulation of plastic flow in a single crystal of pure copper oriented for duplex slip at room temperature ($y_c = 3$ nm in that case). They bear on the spatial distribution of the mobile and immobile dislocations on each active slip system, on the evolution of the dislocation microstructure and of its arrangements, on the evolution of the local and average of internal stresses during straining and on the stress vs. strain curve of the simulated specimen. Further possible developments will be discussed, which involve in particular the introduction of obstacles to dislocation motion, such as clusters of impurity atoms or precipitates, the study of microstructures in creep and in cyclic deformation, the comparison between the stress-strain curve of a free single crystal and that of a single crystal embedded within a surrounding matrix.

EFFECTIVE TENSORS FOR MIXTURES FOR ELASTIC AND ELECTROMAGNETIC PROBLEMS

A.V. CHERKAEV

A.F.Ioffe Physico-Technical Institute
USSR Academy of Science
Leningrad, USSR

(Abstract not available at the time of print)

FLOWS WITH COHERENT STRUCTURES: APPLICATION OF RANDOM POINT FUNCTIONS AND STOCHASTIC FUNCTIONAL SERIES

C. I. Christov

Laboratory of Hydrometeorological Informatics, Hydrometeorological Service, Bulgarian Academy of Sciences, boul. Lenin 66, Sofia, 1184, BULGARIA

ABSTRACT

In recent years a new point of view on turbulence has evolved in the literature according to which along with the small-scale chaotic motions the turbulence signal consists also of organized in a sense (called "coherent") structures with deterministic average shape. Occurrence of coherent structures appears to be a general property of nonlinear dynamic systems with chaotic behaviour of solution and is now a well recognized phenomena far beyond the frame of turbulence investigations.

In authors works, a new approach to the random behaviour of nonlinear dynamic systems has been originated assuming that the predominant part of the random solution is represented by a (generally marked) random point function, composed by structures of similar deterministic shape that are randomly located in the region under consideration (time interval, spatial domain, etc.). The latter is a heuristic assumption based on the observation that the instability gives rise to disturbances that develop and eventually decay returning the system approximately in the same initial unstable state and only after that a new disturbance can occur and the scenario is repeated. During its life span a structure is stable to disturbances of the same characteristic length and the secondary instabilities result in smaller-scale disturbances superimposed upon the main one. This notion fits very well in the picture of a turbulent flow with coherent structures and allows one to obtain self-contained models and to predict quantitatively well the multi-point statistical characteristics of the stochastic regimes for a number of nonlinear systems: Lorenz system, Burgers and Kuramoto-Sivashinsky equations, plane mixing layer, near-wall region of plane Poiseuille flow.

A generalization of the technique is outlined developing the sought solutions into Volterra-Wiener functional series with a marked random point basis function. The higher-order kernels of the Wiener functionals are interpreted as the shape functions of double, triple, etc., interactions among the coherent structures. Upon acknowledging the viriality of the series under consideration a natural way to truncate the infinite hierarchy for kernels is proposed.

A COMPLETE LIST OF INVARIANTS FOR DEFECTIVE CRYSTALS

C. DAVINI * & G.P. PARRY †
* Istituto di meccanica teorica ed applicata,
viale Ungheria, Udine, Italy.
† School of Mathematical Sciences, University of Bath,
Claverton Down, Bath BA2 7AY, England

Burgers' vector and the dislocation density tensor have a geometrical significance which accounts for their predominant position in discussions of the theory of continuous distributions of dislocations. Thus the closure failure of circuits and surfaces is measured by certain of their components, and the dislocation density tensor can be interpreted as the torsion in a non-Riemannian geometry. When these objects are non zero, it is common to say that the corresponding material is defective, so to regard the Burgers' vector and the dislocation density tensor as measures of defectiveness.

This practice can be given a systematic flavour. To begin with, note that the closure failure of a circuit is additive with respect to the composition of circuits defined in the obvious way. Also, closure failure is an elastic invariant in the sense that the Burgers' vector is left unchanged by any elastic deformation of the material if the lattice vectors as presumed to behave as material vectors in the deformation. Analagous remarks apply to the dislocation density. The two objects, then, are additive elastic invariants; they reflect prejudices which require that a measure of defectiveness should

i) mimic the atomistic notion of counting dislocations or vacancies,

ii) be compatible with what might be called "Taylor's conjecture", that a change of defectiveness induces anelastic deformation.

It is generally not acknowledged that there are other objects with these two properties, equally able to measure defectiveness according to the criteria (i) and (ii), likewise admitting persuasive geometrical interpretation. Moreover, knowledge of the fields of Burgers' vectors and dislocation density is generally insufficient to determine these rogue objects, so that the search for an exhaustive list is important.

Now in the theory of discrete dislocations there is a rather specific and common mechanism which is the passage of a single edge dislocation through a perfect crystal lattice, along a specific lattice plane. The motion regenerates the body of the lattice, but there is a relative slip of atoms in the appropriate glide plane. There is a change of shape of the body (the dislocation travels to the boundary) and atoms are displaced, but locally the lattice structure is unchanged in the interior. In the search for a definition of defectiveness with which to assess the utility of any list of additive elastic invariants one must admit, surely, that if the lattice structure is unchanged then so is "the defectiveness". It requires only an acceptance of Taylor's conjecture to deduce that if lattice vectors in two states are related elastically, then the defectiveness in the two states is the same. Loosely, we define two states to be equidefective if, given any two corresponding points in the two states, lattice vectors is a neighbourhood of one of the points are mapped by elastic deformation into the lattice vectors in some neighbourhood of the other point. If one accepts that elastic deformations do not change defectiveness, it is hard to see a way to make a notion of equidefectiveness any more stringent than this.

We define a list of additive elastic invariants to be complete if states where corresponding densities take prescribed values are equidefective. This definition is meant to reflect the idea that a list of invariants is sufficiently descriptive of the defective state if knowledge of those invariants determines the primitive fields to within elastic deformation, locally.

In the context of a continuum model of a crystal where fields of lattice vectors and mass density are regarded as the primitive quantities (1), one of us has derived a list of additive elastic invariants which is exhaustive in that it contains all such objects which are also such that corresponding densities depend only on first derivatives of the primitive fields. The list of invariants in (1) is not complete; here we extend the list of (1) to provide a complete list, and this extension has the additional merit that it removes the need for some non-local analysis that featured in that work. Also, states with prescribed densities are characterised explicitly, and are shown to be related to each other by some kind of "slip" of the lattice vector fields. Since the notion of slip is perhaps the most common and fundamental idea which occurs in phenomenological theories of plasticity, it is at least encouraging to find that it emerges quite naturally from general assumptions which do not anticipate any ideas about the kinematical nature of defectiveness.

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CONSTITUTIVE EQUATION OF A YIELD STRESS FLUID WITH A FROZEN MEMORY, BASED ON THE NETWORK THEORY

P. DOREMUS AND J.M. PIAU

Institut de Mécanique de Grenoble
B. P. 53 X, Domaine Universitaire
38041 Grenoble Cedex FRANCE

Summary : A structural constitutive equation, based on the network theory and on a creation and failure mechanism of junctions is presented in this paper. It allows the behaviour of a class of yield stress fluids to be modelled. A general formulation allows the material functions and the birefringence for two dimensional homogenous flows to be expressed. The problem of initial state is treated. The constitutive equation is then developed on the basis of experimental results and the properties of the model are analysed in detail for explicit adapted forms of junction evolution laws. It can be seen that the model obtained is useful for defining the experimental procedures to be applied in order to characterize yield stress fluids. Finally, a phenomenelogical expression, associated with the constitutive equation is established. It reveals the anelastic behaviour of a material with a non fading memory, and the mechanism of the frozen memory is discussed.

MICROSTRUCTURAL ORIGIN OF HYSTERESIS AND APPLICATION TO CONTINUUM MODELING OF SOLID BEHAVIOUR.

D. Favier [(1)], P. Guélin [(2)], F. Louchet [(3)],
P. Pégon, [(4)], A. Tourabi [(2)], B. Wack [(2)].

(1) Gênie Physique et Mécanique des Matériaux - B.P. 46 - 38402 Saint Martin d'Hères Cédex - Fr.
(2) Institut de Mécanique de Grenoble - B.P. 53X - Grenoble Cédex - Fr.
(3) Laboratoire de Thermodynamique et de Physico-Chimie Métallurgique - B.P. 75 - 38402 Saint Martin d'Hères Cédex - Fr.
(4) Joint Research Center - C.C.E. - 21020 ISPRA (Varese) - It.

The study of metals and metallic alloys behaviour at the macroscopical scale shows that these materials are subjected to many phenomena like viscosity, hardening, softening, hysteresis, aging, damage, ... which are related to a great number of microstructural processes. At room temperature the experimental results indicate that the hysteresis phenomenon is the leading one. A complete description of this behaviour introduces then a scheme of discrete memory type, for the mechanical aspects as well as for the thermodynamical aspects.

The main properties of the discrete memory scheme may be recognized, after stabilization of the hardening phenomena, with "symmetrical" cyclic loading of "unidimensional" type. It consists, for example, in the comparison of four different loading branches going through the origin : first loading branch (1), branch after an inversion at the origin (2), branch passing through the origin (3) and inversion points locus of the fundamental cycling (4). Of special interest is the curve of type 2 obtained by the description of a small cycle into a large cycle : the slope discontinuity, observed after the inversion at the origin, can only be due to the (discrete) memory of a particular event.

An explanation of such results may be obtained at the microscopical scale, where the dislocation movements take place, by considering the elementary mechanisms which are responsible for the deformation. Thus for example the behaviour of a dislocation moving between two parallel walls is equivalent to the behaviour of a couple of a spring and a friction-slider. A second example is represented by a Frank-Read source, operating between two parallel walls, which is equivalent to two couples of springs and friction sliders : the friction sliders are characterized by the values S1 and S2 of the external stress for which the dislocation pinning point moves along the wall and the source emits a dislocation loop respectively.

In a real material there exists an infinity of such elementary mechanisms and the macroscopical deformation is the result of all the area sweeped by the dislocations. The characteristic values Si of the elementary mechanisms are widely dispersed due to their types, dimensions and orientations with regard to the "external" forces, thus explaining the existence of a smooth non linear first loading branch and a similar feature for the unloading and reloading branches. Finally all the macroscopical rate independent properties of pure hysteresis type may be explained in microscopical terms.

CONTINUUM MODELS OF AMORPHOUS AND POLYCRYSTALLINE FERRO-MAGNETS:

MAGNETOSTRICTION AND INTERNAL STRESSES

M. Fähnle, J. Furthmüller and R. Pawellek, Institut für Physik, Max-Planck-Institut für Metallforschung, Heisenbergstr. 1, 7000 Stuttgart 80, F.R. Germany

The paper presents continuum models for the description of amorphous and polycrystalline ferromagnets within the framework of the linearized theory of elasticity. The calculations are based on the incompatibility method introduced by H. Reissner and further evaluated by E. Kröner in his continuum theory of dislocations. Two examples for incompatibilities are discussed, the one introduced by the spontaneous magnetostrictive strains in random ferromagnetic systems as well as the structural incompatibilities inherently related to the amorphous structure. For the first example we are able to characterize for the first time the inhomogeneous nature of the magnetostrictive deformations. Furthermore, we calculate iteratively the macroscopic magnetostriction tensor of amorphous and polycrystalline ferromagnets on a line similar to the theory of random media elasticity of E. Kröner. For the case of internal stresses due to structural incompatibilities we compare our results with the ones derived by Egami and co-workers from computer simulations for the atomic level stresses in amorphous systems.

RANDOM DISPERSIONS OF SEDIMENTING SPHERES

F. Feuillebois
Laboratoire d'Aérothermique, C.N.R.S., Meudon, France.

Recent theories have been concerned with the behaviour of random dispersions of small solid spheres sedimenting in a viscous fluid. A review of the main calculation methods and results is presented, together with some experiments. The different topics are the following:

(i) The calculation of the interactions between two sedimenting spheres (Jeffrey and Onishi 1984, Cichoki et al. 1988). This topic is a prerequisite to the interactions between many spheres in a dilute dispersion.

(ii) The calculation of the interactions between three or more (up to 64) sedimenting spheres, and the relative trajectories of the spheres for some special cases (Masur and Van Saarlos 1982, Caflish et al. 1988, Hassonjee et al. 1988).

(iii) The calculation of the average velocity of sedimentation in a homogeneous dilute dispersion of N spheres (N is large); "dilute" meaning that only pair interactions are considered (Batchelor 1972, 1982, Batchelor and Wen 1982, Cichocki and Felderhof 1989). Recent experiments by the author and collaborators use X-ray absorption to allow measurements in the bulk of the suspension, in regions where the suspension is homogeneous. A consistent comparison to the theories valid for homogeneous dispersions is then possible.

(iv) The calculation of the average velocity of sedimentation in a dilute dispersion which is inhomogeneous along the vertical (Feuillebois 1984).

(v) The question is raised of the influence of the walls of the container on the average velocity of sedimentation (Masur and Beenaker 1985, Nosieres 1987). This section also includes the Boycott effect.

(vi) Another problem is the expression for the variance in the velocity of sedimentation, in view of the available theoretical (Caflish and Luke 1985) and experimental (Ham and Homsy 1988, Davis and Hassen 1988) results.

(vii) Finally, the instabilities observed in bidisperse systems are mentioned together with some proposed explanations (Batchelor and Van Rensburg 1986, Cox 1987).

STRUCTURAL TURBULENCE

M.A.Goldshtik

Institute of Thermophysics, Novosibirsk 630090, USSR

It seems today that classical statistic approaches are inconsistent for construction of kinetic theory and thermodynamics of turbulence. The reason is, as experimental observations show, that quasi-deterministic coherent structure plays a great role in the turbulent transfer processes. Therefore a perspective theory of structural turbulence has to include a procedure of consequent finding and describing the structures and separation of deterministic and stochastic component of turbulent motion. Special dynamical equations are to be obtained for the coherent structures, and some kinetic equations for separated stochastic variables. Though there is an hierarchy of structures, in some simplest cases monostructural approach may be developed. It often happens that when a structure appeares as a result of bifurcation, it is a soliton wave with some known parameters. So a bifurcation of stochastic regime in the Lorenz system related to a breakdown of a separatrix loop, for which the trajectory is a soliton. In supercritical parameter region the trajectory consists of a sequence of solitons appearing with chaotic signs and after chaotic time intervals. This is an example of monostructural chaotic process. Our calculations show that for finding the main moments with a rather good approximation one do not need the kinetic equation, using some simple statistic hypothesis, for example, that each sign is independent variable having values - I and I with equal probabilities. Using this approach we have calculated the soliton profile, the mean time interval between the solitons, the power spectrum for rather wide range of the Rayleigh number.

Using some ideas and methods the strange attractor theory, the method of experimental data analysis have been developed. It allows to find coherent structure in a turbulent signal with the help of some modification of conditional sampling method.

Some structural models were constructed for turbulent flow in a plane channel at near-critical Reynolds numbers, for transition region in boundary layers, for viscous sublayer of near-wall turbulent flows, particularly, for flow of delute polymer solutions. Nonlinear oscillations with structural patterns have been calculated for jetlike flows.

Variational method for fluid mixtures of grade n

Henri GOUIN

Faculté des Sciences et Techniques,
Département de Mathématiques et Mécanique, Case 322
Avenue Escadrille Normandie-Niemen, 13397-Marseille Cedex 13, France.

We suggest a new systematic method that leads to the equations of motion and energy for fluid mixtures without chemical reaction or diffusion.

The mixture is represented by several distinct continuous media that occupy the same physical space at time t. The used variational principle is applied to a lagrangian representation associated with a reference space for every component.

For classical fluids, the method corresponds to Hamilton's principle in which one makes a variation of the reference position of the particle.

It does not yield new results but the inferred equations are written in a different form that better fits to the study of first integrals for conservative motions.

It is not the same for mixtures. The principle appears far more convenient than method only taking variation of average motion into consideration: it separatly tests every component of the mixture and leads to thermodynamic equation of its motion.

The internal energy is a function of different densities or titres of the mixture. Because of the form of the used principle, one must consider an entropy for every component but for the state of mixture. The total entropy of the system is the sum of the partial entropies.

To consider areas where strong gradients of density occur - for example shocks or capillary layers - the internal energy is chosen as a function of the successive derivatives of densities and entropies. An interpretation of capillarity stress is deduced (rule of Antonov).

Two general cases of conservative motions for mixtures are considered: isentropic motion and isothermal motion.

An important case is the one of *thermocapillary mixtures*. It corresponds to an energy taking into account the gradients of densities and entropies. For compressible mixture, the equations of motion involve a hydrostatic stress tensor.

In the same way as for thermocapillary fluids endowed with viscosity, an additional term that has the dimension of a heat flux may be added to the energy equation. That yields a generalization of Clausius-Duhem's inequality which represents the second law of thermodynamics.

HIERARCHY OF DESCRIPTIONS IN THERMODYNAMICS

Miroslav Grmela

Ecole Polytechnique de Montréal
Montréal, Canada

A single physical system can be modeled by several different dynamical theories. For example, hydrodynamics, kinetic theory, equilibrium thermodynamics and classical mechanics can be used to model a liquid (e.g. water). We recall that each of these models have arisen and can be applied independently of others. Every model represents a different experience and a different insight based on different types of observations and measurements.

The mathematical structure of dynamical theories that expresses their compatibility with equilibrium thermodynamics is identified. The structure consists of a symplectic and a metric structure in the state space of the dynamical theory and a generating functional. The generating functional plays three roles. First, its gradient, after being transformed to a vector by the symplectic and the metric structure, becomes the vector field generating the time evolution in the dynamical theory. Second, the generating functional plays the role of a Lyapunov -function associated with the approach to equilibrium states. Third, the generating functional determines the manifold of the equilibrium states. The equilibrium thermodynamics that is implied by the dynamical theory is formulated as geometry of the manifold of the equilibrium states. This way of expressing the compatibility of a dynamical theory with equilibrium thermodynamics is then extended also to a compatibility of a dynamical theory with another, more macroscopic, dynamical theory. The unified formulation of equilibrium and nonequilibrium thermodynamics that results from this analysis can also be applied to externally forced systems. Illustrative examples are taken from the theory of polymeric fluids.

NON-EQUILIBRIUM MOLECULAR DYNAMICS STUDIES OF THE TRANSPORT PROPERTIES AND THE STRUCTURE OF COMPLEX FLUIDS

S. Hess, D. Baalss, O. Hess, W. Loose, J.F. Schwarzl, U. Stottut, and T. Weider
Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-1000 Berlin 12, W. Germany

Non-equilibrium molecular dynamics provides a tool for the microscopic modelling of transport properties and the analysis of the structure of fluids in the presence of transport processes. The basic features of the method are discussed for a plane Couette flow as an example of a stationary transport process. The calculation of the viscosity and the distortion of the velocity distribution, of the pair-distribution function and the static structure factor is well established for simple fluids [1-3]. Some results are presented for the extension of the method to complex fluids, i.e. molecular gases and liquids, nematic liquid crystals and polymeric melts; where also the flow alignment is analysed, as well as to dense colloidal dispersions and oriented ferro-fluids.

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NDT methods of flaw detection in magnetoelastic materials and their modeling.

R.K.T. Hsieh
Department of Mechanics
Royal Institute of Technology
S-100 44 Stockholm, Sweden

Functional materials, in particular, magnetoelastic materials are developing dramatically. This in turn makes the knowledge and control of material defects an increasingly important factor in the continuous technological and industrial race for higher performing materials. In this respect, nondestructive testing methods for the analysis of defects during and after materials processings have received an ever growing attention.
This paper discusses such nondestructive testing methods for flaws in magnetoelastic materials. Special emphasis is given to eddy current nondestructive testings. It shows how they can be modelled by a quasi-static form of Maxwell's equations. An overview is given of both analytic and numerical approaches to the solution of the describing equations. The paper is illustrated with a number of applications.

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HIERARCHIES AND BOUNDS FOR SCALE EFFECTS IN HETEROGENEOUS BODIES

Christian HUET

Ecole Nationale des Ponts et Chaussées
Centre d'Enseignement et de Recherche en Analyse des Matériaux
1 Avenue Montaigne
93167 NOISY LE GRAND CEDEX

We consider elastic heterogeneous bodies or sets of bodies with same external geometry but made of materials that are not statistically homogeneous spatially. For instance they may involve localized defects, or have dimensions lower than those of the representative volume.

By using a variational reasoning derived form the one used by HILL for its modification theorem (1964), one shows that, from the point of view of the apparent properties, hierarchies can be established between various partitions of one such body submitted to two classical cases of boundary conditions.

Further, depending on the kind of boundary condition involved, two sets of absolute lower and upper bounds are obtained.

One is the effective modulus of the associated statistically homogeneous material. The other is one of the two (REUSS or VOIGT) bounds (first order bounds in the sense of KROENER) also derived by HILL (1964) for such statistically homogeneous materials.

Extensions of these results to the case of general linear viscoelasticity are obtained, through the use of our new pseudo-convolutive minimum theorems, that we recently applied already to extend HILL inequalities to the effective creep and relaxation functions of statistically homogeneous viscoelastic materials.

The results presented here, that make also use of the spatio-stochastic approach that we have introduced a few years ago, provide us with practical means of making prediction on the elastic or viscoelastic behaviours of large structural members with defects and/or gross heterogeneities form two sets of experiments performed on statistically representative stochastic sets of small specimens.

These two sets of experiments must involve two appropriate kinds of boundary conditions.

A HOMOGENIZATION TECHNIQUE
BASED ON HILL'S MODIFICATION THEOREM

C. HUET, P. NAVI and P.E. ROELFSTRA

Ecole Nationale des Ponts et Chaussées, Centre d'Enseignement et de Recherche en Analyses des Matériaux, ENPC-CERAM,
1, Av. Montaigne, 93167 Noisy-Le-Grand Cédex, France

and
Ecole Polytechnique Fédérale de Lausanne, Laboratoire des Matériaux de Construction, 32, Ch. de Bellerive, 1007 Lausanne, Suisse

ABSTRACT

The principle of a geometrico-numerical method for evaluating the effective properties of disordered and semi-disordered materials is presented. It is based on an application of the modification theorem established by R. Hill in 1963 and recalled in the paper.

It is shown how the use of monotonic transformations, for instance by using the tools of mathematical morphology, a microscope and a digital image analyser, makes it possible to transform a complicated real material to slightly modified ones the effective properties of which can be calculated, in some instances analytically but most often numerically. For well chosen monotonic transformations, leading to a "diminished material" and an "augmented material", the calculated effective properties are bounds for the corresponding effective property of the real material. These bounds provide precise evaluations in the cases for which the diminished and augmented materials are close one from the other.

Various domains of application are described. Numerical examples, making use of the numerical technique recently developed by P. Navi in ENPC-CERAM for the evaluation of waves celerities and dispersion curves in periodic heterogeneous media are presented. Comparisons with other techniques are also presented. Other examples are presented for the case of random modified structures, making use of the"numerical concrete" software developed in EPFL by P.E. Roelfstra.

It is shown that the method presented here enables one to overcome various difficulties encountered in the application of the theories of heterogeneous media, for instances in the cases of materials involving continuous granulometry, quasi-order, or porosity.

GEOMETRY AND THERMODYNAMICS OF THE GROWTH OF AMORPHOUS SCTRUCTURES

by
R. KERNER
L.P.T.P.E., Tour 16 E1, Universite Pierre et Marie Curie
4, Place Jussieu 75252 PARIS CEDEX 05, FRANCE

ABSTRACT

The growth of solid structures, both amorphous and crystalline, can be described in terms of progresssive association of some elementary stable configurations which represent well-defined minima of the interaction potential between atoms. The ergodicity of the process should lead to the same statistical properties of the real association and growth in time and the "trajectories" traced in the bulk of the resulting network. Such a hypothesis enables us to deduce the statistical properties of networks from some simple assumptions concerning the energy of elementary configurations and their geometry.

A model is presented, which has been solved in two dimensions. The growth process is described by a system of dynamical equations ruling the variation of probabilities of different elmementary configurations. The overall statistics are found, which correspond to stable or metastable global configurations.

A simplified approach to the thermodynamics of such networks is also presented. The configurational entropy is defined and Kauzmann's paradox discussed. An attempt of application of this approach to the 3-dimensional system formed by SiO_2 is presented, too.

C P N P
[illegible] Yotsukaido City, Chiba-ken, 284 Japan
Telephone 0434-22-2850

CMDS 6

Unified C.M.D.S. Standpoint of the Micro-Physical and Macro-Psycho-Physical Perceptions

by Kazuo KONDO

Abstract

This is part of a furtherance of an idea the author referred to in C.M.D.S.4. It starts with pointing out how apparently with a C.M. terminology one can be epistemologically dealing with a D.S. Being put in terms of expoint coordinates, the geometry of higher order space $K_N^{(M)}$ implicitly involves a quantum concept disclosed through its Zermelo conditions

$$\Delta_K F = \delta_K^1 F, \quad \partial F/\partial t = 0,$$

$$(K = 1, \dots, M).$$

It is also related to the logarithmic Weber-Fechner Law

$$\delta F/F = 1$$

through $\delta F = \Delta_1 F$ that can be proven.

Now that the entire edifice of microscopic physics is being embedded in the geometry of $K_N^{(M)}$ and its multiparametric generalization $K_{L,N}^{(M)}$, here is a unified picture of psychology and physics. The Logarithmic Law is reconfirmed whereas the Power Function Law is recognized only as an approximation for a special case.

The origin of the Euclidean metric is also inherent in the C.M.D.S. compromise, depending on the existence of logon quantum. Three-dimensionality, the tristimulus principle as well, is the lower bound, the relativistic space-time concept being introduced where redundancies above this limit are involved.

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NON-CLASSICAL DIFFUSION THEORY

R. Kotowski [*] , A. Trzesowski [*] , K.- H. Anthony [+]

[*] Institute of the Fundamental Technological Research of the Polish Academy of Sciences, Swietokrzyska 11, PL-00-049 Warsaw, Poland

[+] Universität Paderborn, Theoretische Physik, Warburger Str. 100, D-4790 Paderborn, FRG

The aim of the paper is a generalization of the classical diffusion theory which allows for stationary non-equilibrium states. We start with the mass balance equation. This equation containing the mass density and the diffusion peculiar velocity as two unspecified quantities must be supplemented by an additional relation between these two quantities. The classical diffusion theory, for example, is based on the so-called Stokes relation between the peculiar velocity and the velocity of the chaotic motion where the latter one is totally defined by the destribution of mass taking part in the diffusion process (Fick's law). In this paper Stokes relation is generalized in such a way as to take account of the influence of inertial effects. As a consequence those diffusion processes can be described the kinetic relaxation time of which exceeds a particular observation time.

The problem of a Lagrange formulation of the generalized diffusion theory is also discussed.

Dislocations and Chaotic Motions

Isaak Kunin
Department of Mechanical Engineering
University of Houston, Houston, TX 77004

All continuum mechanics theories postulate that a body is a material manifold with topological and differenuable structures invariant under deformations. As a consequence, the equivalence of Lagrangian and Eulerian pictures follows. Elastic deformations and laminar fluid flows are perfectly described as families of diffeomorphisms of materials manifolds.

We argue that this postulate should be critically reconsidered for the motion of dislocations, turbulent flows, and all mixing (chaotic) motions. The only physically justifiable picture for such motions is the Eulerian one. The corresponding mathematical model is based on the geometry of nonholonomic transformations.

Résumé de la conférence invitée au Symposium
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Models and Simulations of Lattice Gases

P. Lallemand
Laboratoire de Physique Statistique
associé au CNRS et l'Université Paris 6
Ecole Normale Supérieure
24 Rue Lhomond
75231 Paris Cedex 05

The purpose of the talk is to present a review of the work performed over the last 4 years since the subject of lattice gas was revived by a proposal of Frisch, Hasslacher and Pomeau[1] of a new way to simulate viscous flows.

In a first part lattice gases will be introduced. They consist in a collection of point particles that move synchronously along the links of a highly symmetric lattice. The dynamics of the lattice gas is decomposed in a succession of two different steps: a *propagation* step during which the particles move from one node to a neighbouring one (often the nearest neighbour or the next nearest neighbour) and a *collision* step corresponding to a redistribution of their velocities according to prescribed rules. In addition the particles satisfy an exclusion principle so that on any node of the underlying lattice there is either 0 or 1 particle with a given velocity. This last assumption leads to great simplifications in the practical use of lattice gases but leads to some unusual physical properties, in particular the lack of galilean invariance.

The macroscopic properties of lattice gases can be derived using general techniques of statistical mechanics in which one deals with particle distribution functions that describe the mean statistical properties of the system. This will be summarized in the second part of the talk which will first indicate how one may obtain an equation of state. Then it will be shown that provided some assumptions can be made concerning higher order particle distribution functions an equivalent of the Boltzmann equation can be written, from which one may derive a Navier-Stokes like equation and determine theoretical expressions for the transport coefficients. Requirements on the choice of the lattice gas will be indicated in order to obtain an isotropic behaviour and to satisfy galilean invariance. A general formula[2] for the shear viscosity of a lattice gas will be discussed with the maximization of the Reynolds number in mind.

The third part will present results of computer simulations of some simple situations. For this purpose various interactions of a lattice gas with a solid boundary will be introduced in order to represent different kinds of boundary conditions. Good agreement with actual experiments will be reported provided similarity rules are correctly used.

The last part will present extensions of the original triangular lattice gas of Frisch, Hasslacher and Pomeau suitable for two-dimensionnal flows of pure fluids to more general cases : three dimensional[3], fluid mixtures with or without sharp interfaces[4], thermal convection[5], application of external fields, etc.... This will include a discussion of the balance between requirements for using simple models that can be implemented on special purpose computers like cellular automata and more elaborate models that possess richer potentialities to represent a larger number of physical situations but require a computer able to perform more elaborate computations.

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SOUND VELOCITIES AND ELASTIC CONSTANTS OF POROUS CERAMICS

H.M. Ledbetter*, M. Lei*, and S.K. Datta**
*Institute for Materials Science and Engineering, National Institute of Standards and Technology, Boulder, Colorado 80303
**Department of Mechanical Engineering and CIRES, University of Colorado, Boulder, Colorado 80309

ABSTRACT

Using theoretical models, we consider the sound velocities and elastic constants of ceramics containing pores. As an example, we consider alumina. However, the approach applies to all ceramics. As a point of departure, we consider spherical pores. For all the usual elastic constants--Young modulus, shear modulus, bulk modulus, Poisson ratio--we give relationships for both the forward and inverse cases: predicting the porous ceramic properties and estimating the pore-free ceramic properties. Following a suggestion by Hasselman and Fulrath that sintering or hot pressing can produce cylindrical pores, we derive a relationship for the elastic constants of a distribution of randomly oriented long cylinders ($c/a = \infty$, the prolate-spheroid limit). This model predicts elastic constants lower than for spherical pores, but well above observation. We obtain agreement with observation by assuming the pores are oblate spheroids. For alumina, the necessary aspect ratio equals one-ninth. Besides pore aspect ratio, the model requires only the pore-free alumina elastic constants. It contains no adjustable parameters.

DUCTILE FRACTURE IN A MATERIAL CONTAINING TWO POPULATION OF CAVITIES

J.B. LEBLOND and G. PERRIN

LABORATOIRE DE MODELISATION EN MECANIQUE
UNIVERSITE DE PARIS VI
TOUR 66
4, PLACE JUSSIEU
75252 PARIS CEDEX 05

The yield criterion proposed in 1977 by A.L. GURSON to model the macroscopic behaviour of a Von Mises material containing voids of identical sizes is now broadly accepted. Nevertheless there is some experimental evidence that in fact cavities of very different sizes coexist. B. MARINI et al. suggested in 1985 that the existence of small cavities scattered between the large ones could modify the final coalescence of the latter. The subject of the present work is to investigate these effects of interaction between two populations of voids of very different sizes.

The present work is based on an explicit solution to the following problem. A hollow sphere made of rigid plastic porous material which obeys GURSON's criterion accounts for one large void surrounded by many small cavities. The calculation supplies the value of the macroscopic flow stress under hydrostatic loading, and the growth rate of the cavities as a function of position.

Two important results are found :

1 . the macroscopic criterion is almost the same as that for a material with only one population of identical cavities that has the same total void volume fraction ;

2 . the growth rate of the small cavities, normalized by that of the central hole, depends on their position : far from the central hole, it is equal to 1, but in the neighbourhood of the central hole, because of interaction effects, it reaches a maximal value of 2.

Point 2 implies that the local porosity close to each large hole grows very fast and can reach the critical value for coalescence before the porosity of the larger holes does. This suggests that the mecanism of damaging could in some cases consist of three successive stages :

1 . the porosities of the two populations of voids grow smoothly ;

2 . close to the large cavities, the porosity of the population of small cavities reaches the critical value for coalescence, and a ring of ruined matter loosens from the porous matrix ; this phenomenon accelerates significantly the growth of the large voids ;

3 . the material is eventually ruined when the large cavities coalesce.

The calculation is used as a basis to develop a simplified macroscopic model that accounts for this behaviour.

FINGERING IN 2-DIMENSIONAL POROUS MEDIA: EXPERIMENTS, NETWORK SIMULATORS AND STATISTICAL MODELS.

Roland LENORMAND

Institut Français du Pétrole
B.P. 311 92506 Rueil Malmaison Cedex. France

This study presents some *discrete* models used to describe the displacement of one fluid by another one in a large network of interconnected capillaries.

Immiscible displacements in porous media with both capillary and viscous effects can be characterized by two dimensionless numbers, the capillary number C which is the ratio of viscous forces to capillary forces and the ratio M of the two viscosities. For certain values of these numbers, either viscous or capillary forces dominate and displacement takes one of the basic forms: (a) viscous fingering, (b) capillary fingering or (c) stable displacement.

The first part of this study presents the results of network simulators (100×100 and 25×25 pores) based on the *physical* rules of the displacement at the pore scale.

The second part describes a series of experiments performed in transparent etched networks.

Both the computer simulations and the experiments cover a range of several decades in C and M. They clearly show the existence of the three basic domains (capillary fingering, viscous fingering and stable displacement) within which the patterns remain unchanged. The domains of validity of the three different basic mechanisms are mapped onto the plane with axes C and M, and this mapping represents the "phase-diagram" for drainage.

In the final section we present three *statistical* models (percolation, diffusion-limited aggregation and anti-DLA) which can be used for describing the three "basic" domains of the phase-diagram.

DILUTE SUSPENSIONS WITH NON-HOMOGENEOUS PARTICLE CONCENTRATION

Daniel LHUILLIER

Laboratoire de Modélisation en Mécanique
(UA 229 du CNRS)
Université Pierre et Marie Curie
Paris, France.

What are the equations of motion of a dilute suspension ? If the particle concentration is assumed to be uniform, there are no special difficulties and the suspension behaviour merely reproduces the single particle behaviour. The situation is drastically changed when the suspension, albeit a dilute one, has a non-uniform particle concentration. The caracteristic length over which the concentration changes must be much larger than the distance between particles (we are looking for a continuum model of the suspension). When performing an average over a volume containing many particles, there are always more particles on one side, and consequently more particles "cut" by the boundary on that side. Due to this inhomogeneous situation, the averaging procedure is no more a trivial matter. This problem was considered by Nigmatulin who used a cellular sheme to tackle it : he divided the volume of averaging into cells containing one particle each and distinguished full cells from cells cut by the volume boundary. This partition into two kinds of cells is a pedagogical way to present the problem but does not really lead to a transparent solution of it. In this communication we revisit this problem of averaging in the presence of a concentration gradient and we solve it explicitly for the case of spherical particles. Our approach avoids the difficulties of the cellular scheme since it is based on the function of presence $\chi(\vec{r},t)$ of the particles in the averaging volume (the average of χ is the particle volume fraction). We will present results for a non-homogeneous sedimenting suspension and compare them with results recently obtained by Nozieres.

FRACTAL MODELS OF MICROPOLAR ELASTIC PERCOLATION.

Laurent Limat

Laboratoire d'Hydrodynamique et de Mécanique Physique, ESPCI, 10 rue Vauquelin, 75231 Paris, Cedex 05, France.

The percolation model is often used in the theoretical description of the mechanical properties of random materials, such as polymeric gels near the sol gel transition, highly porous sintered powders, and more generally two-phase composites near a connectivity threshold. Until recently, it was commonly believed that the observed critical behavior could be understood by electric analogies, the elastic moduli being the equivalents of the conductivity. In fact, it has been shown that the vector nature and the rotational invariance of the selected microscopic model can deeply modify the observed behavior. However, the numerical simulations of this problem are usually faced with unexpected finite size corrections, which limitate the accuracy obtained on the critical quantities (exponents, universal Poisson ratio). In this paper, we present an alternative approach based on analytical calculations performed on regular fractal structures composed of oriented sites linked by two-bodies interactions. These structures can be viewed as exactly solvable versions of random elastic networks near the percolation threshold. These calculations allow to understand the differences mentioned above between the electric and elastic properties, in terms of geometry of the studied structures. They provide independant estimates of the critical quantities which are in good agreement with available numerical ones. Our calculations also allow to discuss some recent conjectures which relate the elasticity exponents to other exponents known more accurately. It seems that new corrections to these expressions must be taken into account, that can received very simple geometrical interpretations. Finally, we show that the vector nature of the problem and its rotational invariance, impose to take into account six independant exponents, which explain the strong finite size corrections mentioned above. All these results are discussed in the context of the micropolar theory of elasticity, which allows to recover a rough symmetry between the two limiting cases, of a "diluted" solid (high porosity) and a "reinforced" one (rigid inclusions in an elastic matrix).

Continuum model for creep damage of metals

Andrzej Litewka
Technical University of Poznań, Institute of Building Structures,
Poznań, Poland

Phenomenological models of the creep damage and creep rupture of solids are generally the extrapolation of the classical rheology. However, because of the complicated character of a tertiary creep , usually the semiempirical formulae are obtained which can be utilized after determining the numerous constants. The satisfactory agreement of the theoretical predictions and the experimental data is obtained only for some selected materials due to carefuly performed curve-fitting procedure. This approach based on the limited number of experimental data resulted in the opinion that there are some materials where creep rupture is governed by the second invariant of the stress deviator whereas for other materials most significant is the maximum principal stress.

The aim of this study is to formulate the creep rupture criterion based on the assumption that the tertiary creep is the result of the stiffness and strength reduction of the material due to crack and void growth. The current state of the deteriorated material microstructure is described by the second rank damage tensor and the appropriate constitutive equations are derived by employing the tensor function representations. The creep rupture criterion proposed consists of the damage evolution equation and the failure criterion for material with oriented deteriorated internal structure. To illustrate the applicability of the theory proposed the multi-axial creep rupture experimental data for various metals were used. It was found that the influence of the second invariant of the stress deviator, maximum principal stress and the first stress invariant on the creep rupture behaviour depends on many interrelated factors like temperature, time to rupture and stress level related to the material strength.

OVERALL BEHAVIOUR OF GRANULAR MATERIALS THROUGH MICROMECHANICS : A DIRECTIONAL APPROACH

Benjamin LORET L.M.S. Ecole Polytechnique Palaiseau I.M.G. Grenoble

Morteza MEHRABADI Tulane University New Orleans

Mailing address :

_ Benjamin LORET 3 rue de Wattignies 75012 PARIS

Abstract submitted to :

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In the past few years, several attempts to describe the behaviour of granular masses using their microstructure have been presented. So far, they show a major drawback due to the fact that they are not able to describe the evolution of the microstructure during a loading process. It is the purpose of this work to develop a framework that allows for this evolution to take place.

Although the study of polycrystals provides a useful guidance to this analysis, it is clear that local mechanisms of deformation in granular materials are not the same as in crystals. In particular, the notion of contact forces is of utmost importance; also changes of microstructure takes place for quite small applied strain. Furthermore, the popular self-consistent scheme is not relevant for granular materials because of the relatively large void ratio.

The granular materials considered here consist of rigid cylindrical rods of circular cross-sections. In fact, the approach does not distinguish individual rods and proceeds as follows:

1. Unit cell.

First, a unit cell is defined in which a local behaviour is postulated. This behaviour aims at describing the two main mechanisms of deformation, namely plastic slip of two granules over one another and changes of microstructure as a result of both the rotation of contact normals

and the generation and loss of contacts. Conceptually, a unit cell represents an intergranular contact : it is characterized by an orientation and the corresponding contact force. The weighted spatial distribution of unit cells, referred to as fabric, is an essential overall feature of the anisotropy of the granular material.

2. Transition scheme.

The transition scheme from the overall level, at which loading is applied, to the local or cell level is made through simple localization techniques, namely Taylor and modified Taylor averaging. The purpose of the latter is to highlight the directional aspect of the local volume change and its relation to the corresponding contact force. Other transition schemes based on the contact forces are also discussed.

3. Averaging procedure.

Once the local material response has been obtained using steps 1 and 2, the overall response to a given deformation process is defined through an averaging procedure. It must be emphasized that the proposed approach applies to any deformation process.

4. Special features and results.

In this analysis, a particular attention is paid to the initial state of the material. This is necessary because, given an overall state of stress and a spatial distribution of unit cells, one has to find an admissible distribution of contact forces ; this point is of importance since, in general, the given initial conditions do not uniquely determine an admissible distribution of contact forces.

The whole procedure has been coded in a computer program. Special attention has been devoted to the presentation of the results. A number of numerical simulations have been performed. For both biaxial compression and shear tests, the evolution of fabric and contact forces is in agreement with the observed behaviour reported in the literature although the predicted overall response is too stiff. In particular, contacts are created (lost) in the direction of maximum (minimum) overall compressive principal stress. The magnitude of contact forces displays the expected trends.

SURFACE ACOUSTIC WAVES ON ROUGH SURFACES

A. A. Maradudin, Department of Physics and Institute for Surface and Interface Science, University of California, Irvine, CA 92717 U.S.A.

A review is presented of recent work on acoustic excitations localized in the vicinity of a rough surface. Three different kinds of rough surfaces are considered, all of which would be planar in the absence of the roughness: (a) a planar surface with an isolated protuberance or indentation on it; a periodically corrugated surface of a solid or a periodically corrugated interface between two different solids; and (c) a randomly rough surface. The first kind of roughness gives rise to surface shape resonances, i.e. to modes that are spatially localized in the vicinity of the surface perturbation and are characterized by discrete frequencies. The calculation of these frequencies is described, as well as the excitation of these resonances by the scattering of a surface acoustic wave from the surface perturbation responsible for them. Waves localized to the surface can propagate across surfaces of the second and third kinds. The effects of the roughness on their dispersion curves and on their attenuation will be discussed. The scattering of bulk acoustic waves from a randomly rough surface, and its connection to the theory of weak localization, is also described.

ANALYSIS OF RANDOM PARTICULATE MEDIA VIA FACTORIAL FUNCTIONAL EXPANSIONS

Konstantin Z. Markov

Faculty of Mathematics and Informatics
University of Sofia, 1126 Sofia, Bulgaria

Let x_j be the set of random points that characterize the location of inclusions in a particulate medium. The random fields $u(x)$ that appear in the medium in a given physical context, say, temperature, displacement, velocity, etc., are represented as functional (Volterra-Wiener) series with the point-wise input—the density field $\psi(x) = \sum \delta(x-x_j)$ of the set x_j. The series are rearranged so as the so-called factorial fields for the set x_j appear; the obtained series are called factorial. A recent result of the author states that the factorial series possess, for a wide class of sets x_j, virial property. This means that the truncations after the pth tuple term of the factorial series for the field $u(x)$ coincide in statistical sense with $u(x)$ asymptotically to the order n^p, where n is the number density of the set x_j, $p=1,2,\ldots$. A general procedure of identification of the kernels and the basic features of the factorial series are discussed, among them, their resemblance to cluster expansions. Unlike the latter however, the factorial expansions are derived and identified in a rigorous way from the governing equations of the problem under study. The performance of the factorial series is illustrated on several examples, *e.g.*, on the steady-state diffusion problem in a random dispersion of spheres whose sink strength differs from that of the matrix. The classical problem of heat propagation through the random dispersion is discussed as well. In both problems full statistical description of the respective random fields, correct to the order n^2, is obtained in a closed form through the solutions of the respective one- and two-sphere inhomogeneity problems.

EFFECTS OF NONLINEARITY AND DISPERSION ON THE PROPAGATION OF SURFACE ACOUSTIC WAVES

A. P. Mayer and A. A. Maradudin, Department of Physics, University of California, Irvine, CA 92717, USA.

The propagation of weakly nonlinear surface acoustic waves of both sagittal and predominantly shear horizontal polarization on a nonlinear, spatially dispersive semi-infinite elastic medium is investigated. Three mechanisms for the introduction of the spatial dispersion are discussed,

- coating by a thin film,
- discreteness of the underlying crystal lattice,
- surface corrugation.

If the new length scales introduced in this way are small compared to the wavelength of the surface wave, their effect consists mainly in a modification of the boundary conditions for the displacement field. In the first and second case, nonlinear dispersion relations are derived, from which, using a method developed by Karpman and Krushkal' [1], conditions for the formation of envelope solitons and the appearance of self-channeling are established. In the second case, an amplitude dependence of the stop bands for weakly nonlinear waves on a periodically corrugated surface is found. Under certain conditions, the nonlinearity can cause Love waves to become leaky with an amplitude dependent damping constant.

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GREEN'S OPERATOR FOR THE DETERMINATION OF THE EFFECTIVE COEFFICIENTS IN RANDOM MEDIA

P. Mazilu

Technische Hochschule Darmstadt

Abstract

The Green's operator is a strong singular integral operator presenting a local and a non-local part. Substantial simplifications are obtained if the non-local part of this operator is neglected and the Green's operator is approximated by its local part. In such approximations the error depends on the chosen reference medium. A careful analysis put into evidence three particulare cases. These cases correspond to a reference medium havings as effective coefficients a) the arithmetic average of the random coefficients, b) the harmonic average of these random coefficients and c) just the unknown effective coefficient to be determined (self consistent method). Each of these reference media is appropiated for a certain type of heterogeneity. Practical computations validate the first type of reference medium for the aggregates of cubic crystals for example, while the third reference medium is appropiated for heterogeneities produced by an infinite number of succesive fracturations of fractal type.

KINETIC PRESSURE AND UNIQUENESS OF ENTROPY IN A NEW THERMODYNAMIC FORMULATION

M. A. Melehy
Department of Electrical and Systems Engineering
University of Connecticut, Storrs, CT 06269-3157, USA

Since the time of Ancient Greece, pressure has been perceived to be an observable quantity, measurable outside a system. For example, the pressure, $\hbar$, just under a liquid surface is the surrounding pressure. In the 19th Century, that view of pressure was incorporated into thermodynamics. For any multiphase system, for example, the criteria of thermal equilibrium, have been assumed to involve the uniformity of $\hbar$. This condition translates into the uniformity of the chemical potential, μ, which depends on pressure.

In the early sixties, this author attempted to develop a unified theory of electrical conduction in semiconductor diodes. Inspired by an idea first conceived by Maxwell in 1860, and now commonly used in statistical mechanics: the pressure for charged particles was assumed to be the kinetic pressure, P, which is: *(2/3) the thermal kinetic energy per unit volume*. For many systems, P and $\hbar$ can be profoundly different. For example, for water that is in equilibrium with its vapor, $P/\hbar \approx 2.35 \times 10^5$, at 300°K.

Using the kinetic pressure has led to a new connection between Newtonian mechanics and thermodynamics, and in turn to a thermodynamic generalization of Maxwell's (1860) diffusion force, f_d. But then an important question arose: how would f_d interact, in any system containing interfaces, with electric, magnetic, and gravity fields, so that the state of thermal equilibrium would be characterized by the principle of microscopic reversibility, as prescribed by its founders (Wegscheider 1901, Einstein 1917, Richardson 1924, Tolman 1925, Lewis 1925)? Answering the above basic question has led to the evolution of the thermodynamic formulation of generalized fields† *(TFGF)*.

The TFGF was applied to semiconductor diodes and solar cells. Theory has accurately been corroborated by experimental data reported by some 35 authors in the period 1951-1987.†

An important question of general interest can now be raised: *has the concept of kinetic pressure accidentally led to correct results for the special case of semiconductor diodes, or is it a universal thermodynamic quantity, that underlies a new formulation, and is waiting to be discovered?* In answering that question, a new connection between quantum mechanics and thermodynamics will be encountered. Specifically, the Gibbs-Duhem equation, which is a consequence of the first law as described by the Gibbs equation, will be solved for pressure, $\mathcal{P}$. The solution involves integrating at constant temperature, T, of the particle concentration, n, with respect to μ. Such an expression for $\mathcal{P}$ should be of significance only if there would exist a way of expressing n as an exclusive function of μ and T. That unique fundamental way had to await the advent of the quantum theory in this Century. Evaluating $\mathcal{P}$, quantum mechanically, it will be shown that $\mathcal{P}$ is the kinetic pressure, P. Extending the techniques further, it will be shown that, in fact, the use of the kinetic pressure provides a necessary and sufficient condition for the uniqueness of entropy, which is required by the second law of thermodynamics.

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MATERIALS WITH THERMOPLASTIC MEMORY

Milan Mićunović
Svetozar Marković University, Kragujevac, Yugoslavia

A geometric description of a crystalline solid body is given by the total compatible deformation represented by means of incompatible thermoelastic as well as plastic deformation tensors (i.e. distortions). They are replacement-invariant in the sense of Dashner.

The principle of determinism is treated here in such a way that elastic response is instantaneous while material remembers temperature history as well as plastic deformation history represented by the asymmetric (second rank) plastic distortion tensor. Frame indifference and material symmetry requirements further specify the functional bringing it into a Lagrangean form.

Materials of integral as well as differential type originating from the above representation are then discussed in detail. Materials of differential type are shown to be elastic-viscoplastic materials. Constitutive restrictions on their inelastic behaviour are derived by extended irreversible thermodynamics and Liu's theorem. So obtained viscoplasticity theory has a non-associate flow rule for plastic stretching and plastic spin tensors. Some recent experiments confirm such a non-associativity /1/. For these evolution equations general tensor function representations for initially isotropic materials are used. Finally, a connexion with some other viscoplasticity theories is briefly discussed.

1. C. Albertini, M.Mićunović and M.Montagnani : Biaxial Strain-Rate Controlled Viscoplastic Experiments on Cruciform Specimens of AISI 316 H up to 100/s, FOURTH INTERNATIONAL CONFERENCE ON MECHANICAL PROPERTIES OF MATERIALS AT HIGH RATES OF STRAIN, Oxford, 20 - 22 March 1989.

BOUNDS ON THE ELASTICITY TENSOR OF ANISOTROPIC TWO-PHASE COMPOSITES

Graeme W. Milton

Courant Institute of Mathematical Sciences
251 Mercer Street, New York, N.Y., 10012

Abstract

Composite materials constructed from two isotropic phases display a range of elastic properties according to the geometrical configuration of the phases. When the composite is isotropic the effective elasticity tensor satisfies the well-known Hashin-Shtrikman bounds on the bulk and shear moduli. The bounds on the bulk modulus are attained by composite sphere assemblages while the bounds on the shear modulus are attained by hierarchical laminate microgeometries. We will discuss various generalizations of these bounds to anisotropic composites. The bounds can be derived either from variational principles or from the more recently developed translation method, also known as the method of compensated compactness. The latter method is more powerful because it yields sharp bounds over a larger range of parameter values. The laminate microgeometries that attain these bounds will be described.

A Note on Periodic and Solitary Wavelike Solutions of the Intermediate Long Wave Equation

Touvia Miloh
School of Engineering
University of Tel-Aviv, Israel

Abstract

The intermediate long wave (ILW) equation is an important non linear integro-differential equation which governs the evolution of long internal waves in a stratified fluid of "finite" depth. It reduces to the Korteweg-de Vries (KdV)[1] and to the Benjamin-Ono (BO)[2,3] equations for "shallow" and "deep" depths respectively. Solitary wave solutions of the ILW equation are well known,[4] however analytic expressions for periodic solutions of the same equation do not seem to exist. Such expressions are derived in this paper and an amazing property discovered for these periodic waves is that they can be represented as an infinite sum of spacially repeated solitons. Thus, *nonlinear* periodic solutions of the ILW equation are obtained by *linear* superposition of solitons. This paper may be also considered as a generalization of the previously known periodic solutions of the kdV[5] and BO[6] for the more general ILW equation

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6th SYMPOSIUM ON CONTINUUM MODELS OF DISCRETE SYSTEMS

Continuum descriptions of polyelectrolyte solutions

Angelo MORRO

DIBE - Università, Viale Causa 13, 16145 Genova, Italy

Abstract

The paper investigates two problems arising in the physics of polyelectrolyte solutions. First, the distribution of counterions around the macroion in a cylindrical cell is examined. A variational formulation is set up an then a numerical method is applied to determine the charge density field in the cell. In this approach the dielectric permittivity is allowed to depend on the electric field. Second, a model for the diffusion in polyelectrolyte solutions is elaborated which incorporates orientational forces dependent on the gradient of the stretching tensor. The model is framed within the thermodynamic theory of miscible mixtures.

REMARKS ON CONTINUUM MODELLING OF FLUID INTERFACIAL REGIONS

A. I. Murdoch
Department of Mathematics
University of Strathclyde

In general fluid interfacial regions are extremely thin and well-modelled as bidimensional continua which can exchange mass with contiguous bulk phases. In this work the problem of motivating bidimensional macroscopic balance relations for interfaces is addressed from a microscopic viewpoint. Specifically considered are the delineation of interfacial boundaries, the notion of interfacial velocity, balances of mass and linear momentum, and the physical interpretation of quantities involved in terms of space-time averages.

VARIATIONAL PRINCIPLES IN THERMODYNAMICS OF DISCRETE SYSTEMS

W. Muschik

Institut für Theoretische Physik, Sekr. PN 7-1
Technische Universität Berlin, Straße des 17. Juni 135
D-1000 Berlin 12

Starting out with global formulations of balance equations and of the dissipation inequality a variational principle for a discrete system in an equilibrium environment is formulated. Applications of this principle to equilibrium conditions of discrete systems and to LANDAU theory of coexisting phases are discussed.

ULTRASONIC WAVE INTERACTION WITH LAYERED ANISOTROPIC MEDIA

Adnan H. Nayfeh
University of Cincinnati
Cincinati, Ohio 45221

ABSTRACT

A unified treatment is presented for the interaction of ultrasonic waves with layered anisotropic media. Our advancements in this field have been motivated by applications in critical systems such as geophysical exploration, transducer design and non-destructive evaluation. Common to all of our studies, is the exact account of the interactions among the layers which manifest themselves in the form of reflection and transmission coefficients. These interactions give rise to geometric dispersion, and depend among other factors, upon the direction of layering and propogation. frequency, the number and nature of interfacial conditions, and above all on the material anisotropy. The most severe consequence of anisotropy is the loss of pure wave mode for general propogation direction. This gives rise to severe complications in the analytical modeling of the propogation process. In our recent studies we have developed techniques which helped us execute our results in closed form simple fashion. In our work, we have been able to overcome these difficulties by recognizing the fact that the wave vectors of the incident and reflected waves must all lie on the same plane. This is a consequence of satisfying appropriate boundary conditions. We therefore conduct our analysis in a coordinate system formed by incident and interfacial planes rather than by material symmetry axis.

Typically, in our studies, we assume a plane acoustic wave to be incident at some frequency, angle of incidence, and azimuthal angle from a liquid upon a multi-layered medium. Each layer is allowed to possess as low as monoclinic symmetry. Reflection and transmission coefficients as well as distributions of displacements and stresses are derived, and from these all propogation characteristics are identified. Solutions are obtained for the individual layers which relate the field variables at its upper and lower surfaces. The response of the total system, proceeds by using the matrix transfer method resulting from satisfying appropriate interfacial conditions across the layers. This model will be compared with extensive experimental results on a variety of composite plates as representative of anisotropic media.

SOME PROBLEMS OF THERMOELASTIC DIELECTRICS

J.P. NOWACKI
IFTR - PAN
WARSAW, Poland

The constitutive equations for thermoelastic dielectrics with polarization gradient have been obtained in an alternative way. The first law of thermodynamics as well as the Clausius-Duhem inequality are used to obtain these equations. On the basis on this theory particular problem is considered. An infinite circular cylinder is held at constant temperature ; the remaining part of material, which fills up the full space, is held at constant temperature, lower than that of the cylinder. The material is thermally stressed and the displacement, temperature and electric fields are calculated. The electric displacement identically vanishes everywhere as it should in absence of free charges. It has been shown that the polarization and electric fields are continuous across the surface of the cylinder, while their first derivatives suffer a jump. For the Cauchy stress tensor, the normal component is continuous, while tangential components are discontinuous.

PERCOLATION, FRACTALS, AND ENTROPY OF DISORDER IN DAMAGE PHENOMENA*

Martin Ostoja-Starzewski
School of Aeronautics and Astronautics
Purdue University
West Lafayette, IN 47906
USA

This paper focuses on the modelling of damage phenomena in solids with random granular microstructures. Damage is defined as an elastic-inelastic transition in the grain boundaries, whereby inelasticity signifies plasticity and cracking. Representation of the microstructure in terms of a graph G [1], permits modelling of intergranular damage in terms of a ternary random field Z on the Graph G' dual to G. Accordingly, the boundary in the stress space between elastic and inelastic response ranges is given by a statistical family of random failure surfaces, and the problem of determination of a macroscopically effective failure surface is reduced to the problem of percolation of inelastic phases on G'[2]. Results of the percolation theory applied to our problem bring out naturally the size effects - decrease of scatter in strength with specimen size and dependence of average strength on specimen size - as well as the fractal character of percolating sets of inelastic phases. Indeed, the field Z represents a multifractal, and this establishes a connection with the findings of Williford [3] on the relation of distribution of microfracture energies to the distribution of fractal dimensions of fracture surfaces.

On the other hand, a direct link is found between the entropy of disorder of field Z and the thermodynamic entropy. This leads to a random scale-dependent dissipation function of a statistical continuum approximation, randomness disappearing for an infinite specimen size only. With the help of the orthogonality condition, both the stochastic and the average damage equations can then be derived.

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[2] M. Ostoja-Starzewski, "Mechanics of Damage in a Random Granular Microstructure: Percolation of Inelastic Phases", Lett. Appl. Engng. Sci., in press.

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* To be presented at CMDS6, Dijon, France, 1989.

ELECTROSTRICTION OF LIQUID CRYSTALS

Ch. Papenfuß, R. Ellinghaus and W. Muschik

Institut für Theoretische Physik, Sekr. PN 7-1
Technische Universität Berlin, Straße des 17. Juni 135,
D-1000 Berlin 12

Starting out with the balance equations of mass, momentum, moment of momentum and energy for liquid crystals and the Maxwell equations, the dissipation inequality extended by external electromagnetic fields is exploited using Liu's procedure. The state space is spanned by

$$Z = (\rho, T, \underline{d}, \underline{\mathcal{E}}, \underline{B}, \nabla\rho, \nabla T, \nabla\underline{d}, \nabla\underline{v}, \dot{\underline{d}})$$

ρ : density
T : temperature
$\underline{d}$: director
$\underline{E}$: electric field
$\underline{B}$: magnetic field
$\underline{v}$: velocity

$$\underline{\mathcal{E}} = \underline{E} + \underline{v} \times \underline{B}$$

The presuppositions are, that $\partial\underline{Q}/\partial\underline{\mathcal{E}}$ and $\partial q/\partial\nabla T$ are regular. This allows to determine the Liu lambdas and to achieve constraints of the constitutive equations. Electrostriction is described by a relation between $\nabla\underline{d}$ and $\underline{E}$ in equilibrium.

PULSE COLLISIONS FOR COUPLED NLS EQUATIONS

D. F. PARKER

Department of Theoretical Mechanics,
University of Nottingham, Nottingham NG7 2RD., U.K.

In a number of continuum and discrete systems, it has recently been shown that the equations governing modulations of harmonic wavetrains are a coupled pair of nonlinear Schrödinger equations. Examples arise from the analysis of optical fibres and of certain bimodal one-dimensional lattices. In some circumstances, the equations possess sech-envelope solutions having the same form as the 'solitons' of the single NLS equation. However, even in these cases it is exceptional that a collision between two such pulses should be a true soliton collision, producing two emergent pulses identical in form to the incident pulses.

Various physical models leading to coupled NLS equations will be briefly outlined. For certain special combinations of coefficients in these equations, analytic results are available and will be surveyed. The important simplifications resulting from symmetries in the physical model will be emphasized. Besides the special cases in which the system is comletely integrable, these include cases having rotational symmetry about the propagation axis, reflectional symmetry in two perpendicular axes and the 'symmetry of the square'. All these cases allow the propagation of certain sech-envelope pulses having different polarizations. Results of computations of collisions between two such pulses show that frequently two pulses of permanent form emerge, but that commonly these pulses are not sech-envelope pulses.

Using similarity analysis, it is confirmed that a wide range of non-distorting pulses exists. The systems of ordinary differential equations governing these pulses are derived. It is shown that these allow solutions in which each model amplitude may be either even or odd about the pulse centreline. The pulses having a single peak amplitude for each mode are particularly relevant to the collision studies. They are computed and compared to the pulses which are found to emerge from collisions of 'sech-envelope' pulses.

FRACTURE MECHANICS OF COMPOSITE MATERIALS ON ACCOUNT OF THE MICROSTRUCTURE

V.Z. PARTON
Moscow Institute of Chemical Machinery
K. Marx Street 21/4
MOSCOW, USSR, 107884

The stress analysis of strongly nonhomogeneous (composite) materials with the idealized macrocrack is usually based on the transformation of such media to the equivalent (in the sense of mean reaction) homogeneous anisotropic media.

Such an appraoch allows us to reduce the calculation of the mean values of the stress field in cracked composites to the solution of the elasticity problem for the anisotropic media with a mathematical cut. If the material has periodic structure one can find the mean (effective) parameters of equivalent media with the help of the averaging method which gives the asymptotically exact approach to the problem for the nonhomogeneous media. Doing so one can quite exactly analyse the local structure of the fields under investigation. This approach was applied to the analysis of the stress fields near the crack tip in a layered composite with periodic structure.

In some cases the formulae for the stress intensity factors are obtained. Besides this, the more elegant method of the stress intensity factors evaluation in the composite media with cracks was developed. It is based on the averaging method with the account of complementary solutions of the boundary layer type.

Oscillatory and nonlinear convection in an isotropic thermomicropolar fluid.

by

L.E.Payne[(1)] and B.Straughan[(2)]

[(1)]Department of Mathematics,
Cornell University,
Ithaca,
New York 14853,
U.S.A.

[(2)]Department of Mathematics,
The University,
Glasgow G12 8QW,
Scotland.

The Bénard problem for a thermomicropolar fluid is investigated. Attention is focussed on the possibility of oscillatory convection and on nonlinear energy stability. For a certain sign of the thermal interaction coefficient (compatible with the Clausius-Duhem inequality) we are able to fully analyse the problem. A striking feature is that stationary convection is seen to be likely to be the physically realizable mode whereas oscillatory convection is likely to occur only at very high Rayleigh numbers and then only when the layer is heated from above.

6^{th} Symposium on Continuum Models and Discrete Systems. Dijon, June 26-29, 1989

Statistical Mechanics of a Nonlinear Model for DNA Denaturation

M. PEYRARD
Laboratoire ORC : Physique des Excitations Non Linéaires
Faculté des Sciences,
6 blvd Gabriel, 21100 Dijon, France.

and

A. R. BISHOP
Theoretical Division and Center for Nonlinear Studies,
Los Alamos National Laboratory, Los Alamos, New Mexico, USA.

The dynamics of DNA transcription is one of the most fascinating problems of modern biophysics because it is at the basis of life. However it is also a difficult problem due to the complex roles played by RNA polymerases in the process. Is is now well established that a local denaturation of DNA is involved so that it is interesting to investigate the thermal denaturation of the double helix as a preliminary step for understanding the transcription.

In the last few years, the idea that nonlinear excitations could play a role in the dynamics of DNA has become increasingly popular. Several models have been proposed in which kink-shaped solitary waves represent the open states ot the double helix. However the solutions were obtained in a continuum limit, a severe approximation of DNA, and they were not related to thermal denaturation since no statistical mechanics of the models was considered. At the same time, an alternative approach more closely related to experimental data was developped to analyze infrared and Raman experiments. It suggested that local melting could be achieved through breathing modes but the analysis was based on a self-consistent phonon approach, it i.e. an extension of *linear* theories, in spite of the very large motions involved.

We treat intrinsically the nonlinearities in a model similar to those used to analyze the spectroscopic data. The main variable is the stretching of the hydrogen bonds that connect two bases forming a pair in the double helix. The statistical mechanics of this model is investigated with the transfer integral method and we determine, in particular, the temperature dependence of the inter-strand separation.

Using a small amplitude expansion suitable for the analysis if the *initiation* of the denaturation, we show that an energy localization process analogous to *self focussing* in plasmas might explain why the denaturation starts at temperatures significantly lower that one would expect by considering the strength of the chemical bonds connecting the two strands.

OBSERVATION OF ACOUSTIC ENVELOPE SOLITARY WAVES AND ELECTROMAGNETIC SOLITON LIKE PULSES GENERATED BY METALLIC INTERDIGITAL TRANSDUCERS ON A QUARTZ CRYSTAL

M. Planat

Laboratoire de Physique et Métrologie des Oscillateurs du C.N.R.S.
associé à l'Université de Franche-Comté-Besançon
32, avenue de l'Observatoire - 25000 Besançon - France

Amplitude and frequency modulational instability, pulse compression and splitting, FPU recurrence and solitons have already been observed in hydrodynamics, electrical transmission lines, plasma physics and optical waveguides. No such behavior has yet been seen in solid state acoustics at room temperature.

In this paper we show that the bulk acoustic wave radiation from interdigital transducers deposited on a quartz crystal plate is dispersive and nonlinear. Envelope modulation, envelope splitting and compression of the acoustic wave signal are observed when the incident pulse energy is increased by varying frequency, input pulse lenght or amplitude. A rough agreement with a simple theoretical model based on the nonlinear Schrödinger equation is obtained.

In addition it is seen that the electromagnetic wave excited by the transducer is strongly affected at frequencies where the acoustic signal can propagate. Long wave lenght pulse solitons characteristic of nonlinear electrical transmission lines are observed.

We hope that this nonlinear coupling of acoustic and electromagnetic signals offers a good opportunity to study the basic physics of piezoelectricity.

GEOMETRIC METHODS FOR COSSERAT MEDIA

by J.F. Pommaret
Centre de Mathématiques Appliquées (CERMA)
Ecole Nationale des Ponts et Chaussées (ENPC)
La Courtine,93167 Noisy-le-Grand Cedex,France

In 1909,the brothers Eugène and François COSSERAT developped a specific variational calculus based on group theory in order to relate geometry (strain) to physics (stress) in the mechanics of continua with non-symmetric stress tensor. They first wanted to extend to continua the well-known variational techniques of rigid body and analytical dynamics.However,they also wanted to clearly define the concept of "torsor" as a generalization ~~of~~ the concept of "vector" different from that of "tensor",while showing that the form of the static or dynamic equations for stress only depends on the structure of the group involved.They succeeded through tedious computations but François COSSERAT died in 1914 and nothing more has been published afterwards by his brother.

In order to extend this argument by enlarging the group,H. WEYL tried (like J.C. MAXWELL),in 1917,to incorporate electromagnetism in some kind of similar dynamics,but failed though finding the basis of modern gauge theory.

More recently,G. BIRKHOFF in 1954 and V. ARNOLD in 1966 got difficulties when trying to pass from rigid body dynamics (Lie group of transformations) to incompressible fluid hydrodynamics (Lie pseudogroup of volume preserving transformations).

The purpose of our lecture is to prove that all these attempts can only be understood by means of the new group theoretical and differential geometric methods introduced by D.C. SPENCER around 1970 in the formal theory of systems of partial differential equations and Lie pseudogroups (groups of transformations solutions of systems of partial differential equations).

We shall sketch simply these methods and apply them to the study of non-linear field theories (mechanics of micropolar media,thermodynamics,electrodynamics).In particular,we shall obtain the following results:

1) The brothers COSSERAT were just computing the non-linear Spencer operators for the group of Euclidean motions.

2) Thermoelasticity,thermoelectricity,photoelasticity,viscosity and streaming birefringence follow from the above procedure which contradicts the distinction usually made between reversible and irreversible phenomena.

NONLINEAR DYNAMICS AND INSTABILITY OF TWIN BOUNDARIES IN MARTENSITIC-FERROELASTIC MATERIALS

J. POUGET

Laboratoire de Modélisation en Mécanique
Associé au C.N.R.S.
Université Pierre et Marie Curie, Tour 66
4, Place Jussieu, 75252 Paris Cédex 05, FRANCE

Nonlinear dynamics and instability processes of a lattice model for martensitic-ferroelastic transformations are presented. Martensitic ferroelastic transitions can be characterized by an order parameter (depending on temperature) which is mostly a strain connected with the symmetry group of the crystal. The transition from the high temperature phase to the low temperature phase is usually accompanied by the formation of martensitic domains (deformed lattice) consisting of more or less complex patterns. The starting point of the study is the construction of a two-dimensionnal lattice model involving nonlinear and competing interactions. In fact, the lattice distortion proceeds by shearing the close-packed atomic layers stacked in a cristallographic direction leading thus to strongly deformed regions separated by interfaces. On the basis of the lattice model we deduce the nonlinear equations governing the strain in the continuum approximation of a one-dimensionnal reduced version. Because of the special interatomic potentials thus introduced, the continuum model accounts then for nonlinear elastic and weakly nonlocal behaviours. The latter play a predominant role in the propagation of nonlinear excitations of the soliton type. The results are: (i) periodic nonlinear waves corresponding to modulated structures, (ii) arrays of solitons made of periodic arrangements of martensitic-elastic domains and (iii) a martensitic soliton moving in an austenitic matrix (undeformed lattice). Insofar as the very discrete system is considered, the static state and analytic solutions of the discrete equations are formally obtained. The static solution is interpreted as a periodic commensurate or incommensurate structure of tiny martensitic domains.

The complete two-dimensionnal model is examined next. We direct our attention to the instability process of a soliton solution with respect to the transverse pertubations giving rise to a complex dynamics of domain patterns. The analytical study of the lattice stabiblity shows that the instability is closely connected with the phase transition phenomena and depends on the nonlinear elastic potential. Since these problems are somewhat cumbersome, the physical conjectures are checked by means of numerical simulations both for the one and two dimensionnal models with the help, of course, of the system of discrete nonlinear equations.

ELECTRICAL TRANSMISSION LINES AND SOLITON PROPAGATION IN PHYSICAL SYSTEMS (*).

Michel Remoissenet . Laboratoire O. R. C,
Université de Bourgogne, 21100 Dijon France.

Abstract.

Distributed electrical transmission lines are convenient models to study nonlinear wave motion : shock waves, solitary waves and solitons, in many interesting physical systems such as lattices, plasmas, optical devices. They also have direct applications to engineering and modern electronic systems for harmonic generation, pulse shaping and compression, data transmission and coding.
As a remarkable particular case one has the discrete transmission line which models the Toda lattice whith discrete soliton solutions. But generally, the dynamics of other elementary discrete transmission lines must be studied theoretically in the continuum limit via nonlinear partial differential equations. Here, we present the characteristic properties of some specific nonlinear transmission lines, in relation with experimental results on pulse solitary waves and solitons propagation and interaction.

(*) Based on a talk given at the "*6th Symposium on continuum models and discrete systems*". June 26-29. Dijon, France.

PLASTICITY OF FIBRE-REINFORCED MATERIALS

T. G. Rogers
Department of Theoretical Mechanics,
University of Nottingham, England

Abstract

In this paper we consider mathematical theories to describe the elastic-plastic behaviour of composites consisting of a ductile matrix reinforced by one or two families of strong, continuous fibres. The responses of such materials are highly anisotropic, with the fibres defining 'preferred' directions in the characterisation of the material behaviour.

We present constitutive equations to describe small or large deformations, and which incorporate the changing orientations of the fibres and hence of the material's anisotropies.

General yield criteria are constructed, and special useful cases discussed. Non-hardening flow rules are considered, together with some types of anisotropic hardening.

Simple applications of the theory are briefly described in the contexts of torsion of thin plates and of finite bending of beams.

Void Force in Granular Assembly

M. Satake
Department of Civil Engineering
Tohoku University, Japan.

As is already shown, the graph-theoretical approach to the mechanics of granular materials is very effective to clarify the correspondence between quantities in granular assemblies and in continua. The void force is a force (or a couple) defined for each void in a granular assembly by applying the graph-theoretical approach and has a property similar to the stress function in ordinary continua. This paper will give the precise explanation on the void force and show some new analysis of granular assemblies by use of the void force.

Kinetic Theory of Dynamic Strain Aging

J. Schlipf

Institut für Allgemeine Metallkunde und Metallphysik

der Technischen Hochschule Aachen, RFG

Strain aging effects are brought about by the diffusion of solutes to dislocations, if the diffusion time t_a is comparable to the waiting time t_w of the dislocations in front of an obstacle. Under suitable external forces an interplay is established between dislocation pinning and dislocation breakaway. The phenomenon manifests itself in (i) amplitude dependent internal friction (ii) modulated response to cyclic straining, and (iii) serrated plastic flow. Although many ad-hoc-models have been published, no consistent theory of these effects is presently known. In the present paper, after a short review of existing models, a treatment based on a master equation for the aging processes will be proposed. The master equation is constructed from the probability distribution of dislocation segments having a given number of additional pinning points.

This equation is highly non-linear and can be solved only numerically. Nevertheless, the evolution of the non-stationary states far from equilibrium can be demonstrated. The results of computer simulations and comparison with published data will be presented.

RECENT DEVELOPMENTS IN GEOMETRICALLY EXACT (COSSERAT) SHELL MODELS: FORMULATION AND NUMERICAL ANALYSIS

J.C. Simo

Stanford University

Abstract

Over the past fifteen years, contemporary developments in nonlinear analysis, differential geometry and numerical analysis have had a profound impact in nonlinear continuum mechanics. In this lecture, we shall review some recent developments concerning the formulation and numerical analysis of shell theory viewed as an *extensible one-director Cosserat surface model.* The models discussed incorporate large strains, finite rotations, finite thickness changes, and accommodate variable thickness. Numerical analysis and computational aspects relevant to the implementation of these models in the context of the finite element method are also addressed in some detail.

Throughout the lecture, emphasis is placed on the interplay between the numerical analysis and the geometry underlying these continuum models which, from a computational standpoint, leads to the development of rather natural algorithmic procedures. Representative large-scale numerical simulations are presented that illustrate the topics covered in the lecture.

STOCHASTIC APPROACH TO FATIGUE FRACTURE

K. Sobczyk

Institute of Fundamental Technological Research,
Polish Academy of Sciences,
ul. Swietokrzyska 21; 00-049 Warsaw

Abstract

Fatigue process is a complex phenomenon which takes place in structures operating under time-varying loading. Nowdays, the needs of aircraft technology, where fatigue problems are of major concern, have stimulated research work of fatigue fracture of various engineering materials. This research has provided significant advances in our understanding of the fatigue behaviour of real materials as well as throwing some light on the physical and statistical nature of fatigue. Due to the inherent complexity of fatigue phenomena the existing results are, however, for from satisfactory. The question of how to perform a probabilistic analysis of a random fatigue process which would lead to a consistent theory of fatigue remains an important and challenging task today.

In the lecture the problems, methods and results concerned with stochastic modelling of fatigue fracture will be presented. First, the physical and engineering origins of the fatigue phenomenon are briefly outlined. After that, the main existing approaches to random fatigue problems and the models for the fatigue crack growth are described (Markovian evolutionary probabilistic models, randomised fatigue crack growth differential equations, stochastic cumulative jump models). In more details a cumulative stochastic jump model is presented. Parameters of the model can be identified from the appropriate fatigue experiments; it is shown that they can also be related to the quantities occuring in the existing empirical fatigue crack growth equations.

PIEZOELECTRICITY AND HOMOGENIZATION APPLICATION TO BIOMECHANICS

Józef Joachim TELEGA

Polish Academy of Sciences
Institute of Fundamental Technological Research
Swietokrzyska 21
00-049 WARSAW
Poland

Abstract :
The aim of this contribution is to study some homogenization problems posed by piezoelectricity. Particularly, we shall present the results concerning :

1. Homogenization of piezoelectric materials under the assumption of periodicity and quasi-periodicity.
2. Homogenization of fissured piezoelectric materials in the presence of unilateral conditions on fissures.
3. Homogenization of piezoelectric shells.

To perform the homogenization procedure, the method of epi-convergence is used in conjunction with partial duality.

Results obtained for piezoelectric solids will be applied to biological materials possessing piezoelectric properties.

The Plastic Spin : Microstructural Origin and Computational Significance

Cristian TEODOSIU

Laboratoire Génie Physique et Mécanique des Matériaux,
Institut National Polytechnique de Grenoble, ENSPG, bp 46
38402 - Saint Martin d'Hères Cédex, France.

The kinematic description of large deformation plasticity is based on a multiplicative decomposition of the deformation gradient, which is a natural extension of the similar decomposition valid for single crystals. However, a precise significance should be given to the director frame defining the orientation of the intermediate configuration of a polycrystalline volume element. In the present approach, following Mandel, a kinematic definition of this frame is adopted, its spin being taken equal to the average lattice spin of the grains over the polycrystalline volume element.

The resulting formulation is analysed, by pointing out the advantages of this choice. First, a maximum simplification of the description of the thermoelastic response is achieved, because the thermoelastic constants are approximately constant with respect to the frames of the intermediate configurations. Next, and the most important, the normality structure of the plastic or viscoplastic constitutive laws can be transferred from the grain level to the polycrystalline aggregate. In particular, it can be shown that both the plastic strain rate and the plastic spin can be derived from a plastic or viscoplastic potential. Finally, the evolution of the texture appears as the change in the dispersion of the lattice orientation of the crystallites with respect to its mean rotation velocity. The latter, i.e. the plastic spin, incorporates in particular any overall rotation effects.

Specific forms of the constitutive laws can be derived by choosing a particular form of the plastic potential. In particular, by adopting a Bingham model for each active glide system, a micro-macro transition of Sachs type leads to a quadratic potential that generalizes Hill's yield function via a non-symmetric, fourth-order tensor of plastic anisotropy. The evolution equation obtained for this tensor clearly emphasizes the respective roles of the plastic spin and of the texture evolution, and permits to consider them as strain-induced effets in addition to the more classical isotropic and kinematic work-hardening.

A special attention is given to the weak formulation of the boundary-value problems. The computational significance of the plastic spin and texture evolution is analysed within the context of an updated Lagrangian description and illustrated by several numerical examples.

Finally, it is argued that numerical simulations based on various hypotheses of micro-macro transition could be sensibly used to identify the model.

Quasicrystals: Stability und Defects

H.-R. Trebin
Institut für Theoretische und Angewandte Physik
der Universität Stuttgart
Pfaffenwaldring 57, D-7000 Stuttgart 80, F.R.G.

Since 1984 a great number of binary and ternary metallic alloys (e.g. $Al_{0.86}Mn_{0.14}$) have been discovered, whose electron diffraction spectra and morphology display the noncrystallographic icosahedral symmetry. For their structural characterization two rhombohedra are employed – an oblate and a prolate one –, which tile space completely in an aperiodic way and which systematically are decorated with atoms. The resulting arrangements are denoted quasicrystals or Penrose patterns.

In this talk several types of quasicrystals are tested with respect to their stability. First the atoms are endowed with pair potentials. Then in a simulation they are allowed to move into equilibrium positions following their mutual forces. Many diatomic quasicrystals prove stable, but we also discovered a stable *mono*atomic quasicrystal, and stability is preserved even if in the initial state the atoms are displaced randomly by up to 7% of the next neighbour distance. Other types of decorations cause a relaxation to the amorphous state. In a video film it is shown that in the course of the decay families of "Fibonacci-planes" are formed whose separations consecutively are scaled down to atomic distances in a self-similar fashion.

Quasicrystals possess translational symmetry in higher dimensions, which is used to construct dislocations and disclinations. In a second video film it is demonstrated, how dislocations move, being accompanied like polarons by a cloud of additional elementary defects, denoted "phasons". These correspond to the planar discommensurations of incommensurate systems, but in quasicrystals can dissolve into linear strings.

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France

6th SYMPOSIUM ON CONTINUUM
MODELS AND DISCRETE SYSTEMS

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METRIPLECTIC DYNAMICS OF COMPLEX SYSTEMS.

A NEW PARADIGM, OR THE OLD APPROACH IN A NEW GUISE?

Łukasz A. Turski

Institute for Theoretical Physics
Polish Academy of Sciences
Al. Lotników 32/46, 02-668 Warszawa
POLAND

Several research groups have recently proposed a variant approach to the dynamics of nonlinear systems, which encompasses both canonical (reversible) and dissipative dynamics. That seemingly new approach has been called *metriplectic dynamics* and some researchers consider it as a new paradigm of the nonlinear mechanics.

In this lecture I will discuss basic formulation of the metriplectic dynamics and try to answer question posed in the title. In doing so I will use examples from contemporary statistical physics, particularly complex systems with internal degrees of freedom and/or magnetic systems.

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Variational Methods in the Theory of Random Composite Materials

J. R. Willis[1] and D. R. S. Talbot[2]

[1] School of Mathematical Sciences,
University of Bath,
Bath, BA1 7AY.

[2] Department of Mathematics,
Coventry Polytechnic,
Coventry, CV1 5FB.

A variational structure, applicable to a range of nonlinear problems, which reduces to the Hashin-Shtrikman structure in the special case of linear behaviour, will be reviewed. It allows the development of bounds, and variational self-consistent estimates, for the overall potential functions of nonlinear composites whose local behaviour can be described in terms of stress or strain-rate potentials. Mathematically, these composites could equivalently be regarded as non-linearly elastic but subject to geometrically linear strains. The variational structure employs a 'comparison medium' which is to be chosen optimally: in contrast to the linear problem, the 'best' comparison medium depends on the overall level of stress, and may be anisotropic even when the composite itself is isotropic. This is illustrated by constructing a new lower bound for the strain-rate potential (or complementary energy) of an incompressible, isotropic, nonlinear matrix, containing an isotropic distribution of spherical voids: the bound is higher than one previously constructed using an isotropic comparison medium. More generally, a lower bound is constructed for a matrix containing aligned spheroids, including aligned penny-shaped cracks as a limiting case.

Contributors

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1, Place Aristide-Briand - 92195 Meudon Cedex - Tél. 45 34 75 50 - Télex 204135